Dilemmas in Design: From Neyman and Fisher to 3D Printing

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From Neyman and Fisher to 3D Printing

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Abstract

This manuscript addresses three dilemmas in experimental design.

1) The Neyman-Fisher controversy originated in 1935, when Neyman asserted that the ANOVA F-test is valid for randomized complete block designs, and invalid for Latin squares, detecting differentiation among the treatments, when none existed on average, more often than desired. However, his expressions for the expected mean residual sum of squares are generally incorrect. Furthermore, his belief that Type I errors are higher whenever the expected mean treatment sum of squares is greater than the expected mean residual sum of squares is generally incorrect. This controversy had a deleterious impact, with potential outcomes ignored in favor of procedures that are imprecise without applied contents.

2) An important issue in fractional factorial designs is the parameterization of factorial effects. The classical orthogonal components system facilitates calculations of design properties for regular fractions, but has two major disadvantages: it induces a simple aliasing structure, and does not yield substantive interpretations for interactions of quantitative factors. An alternative that yields conclusive inferences and interpretable contrasts is the linear-quadratic system. However, its mathematics are not yet transparent. A better understanding

is achieved with indicator functions, and we develop the theory of indicator functions under the linear-quadratic system. New algebraic operations for calculating indicator function coefficients are defined that facilitate the study of partial aliasing relations. They also yield a new connection between design constructions and their analyses under the linear-quadratic system.

3) Additive manufacturing, or 3D printing, is a promising manufacturing technique marred by product deformation due to material solidification. Deformation control can be achieved by a compensation plan. However, little attention has been paid to interference in compensation, thought to result from the inevitable discretization of a compensation plan. We investigate interference with an experiment involving the application of discretized compensation plans to cylinders. Our treatment illustrates a principled framework for modeling interference by means of graphical posterior predictive checks. Properly defining experimental units and understanding interference are critical for quality control in manufacturing. We provide a step in that direction for 3D printing.

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Citations to Previously Published Work

Chapter 1 is based on a paper that can be found in *Statistical Science*.

Sabbaghi, A. and D.B. Rubin (2014) Comments on the Neyman-Fisher controversy and its consequences. *Statistical Science* in press.

Chapter 2 is based on a paper that can be found in *Biometrika*.

Sabbaghi, A., T. Dasgupta, and C-F.J. Wu (2014) Indicator functions and the algebra of the linear-quadratic parameterization. *Biometrika* doi: 10.1093/biomet/ast070.

Chapter 3 is based on a paper that is under review in *Annals of Applied Statistics*.

Sabbaghi, A., T. Dasgupta, Q. Huang, and J. Zhang (2014) Inference for deformation and interference in 3D printing. *Annals of Applied Statistics* revised and resubmitted.

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Dedicated to my father, the best man that I have ever known.

Only a dad but he gives his all,

To smooth the way for his children small,

Doing with courage stern and grim

The deeds that his father did for him.

This is the line that for him I pen:

Only a dad, but the best of men.

Only a Dad, by Guest (1916, p. 42)

Chapter 1

Comments on the Neyman-Fisher Controversy and its Consequences

1.1 Conflict and Controversy

Prior to the presentation of *Statistical Problems in Agricultural Experimentation* to the Royal Statistical Society in 1935 (Neyman, 1935), Jerzy Neyman and Ronald Aylmer Fisher were on fairly good terms, both professionally and personally. Joan Fisher Box's biography of her father (Box, 1978, p. 262-263, 451) and Neyman's oral autobiography (Reid, 1982, p. 102, 114-117) describe two scientists who respected each other during this time. However, Neyman's study of randomized complete block (RCB) and Latin square (LS) designs sparked Fisher's legendary temper (Reid, 1982, p. 121-124; Box, 1978, p. 262-266; Lehmann, 2011, p. 58-59), with the resulting heated debate recorded in the discussion. The relationship between Fisher and Neyman became acrimonious, with no reconciliation ever being reached (Reid, 1982, p.

124-128, 143, 183-184, 225-226, 257; Lehmann, 2011, Chap. 4).

The source of this conflict was Neyman's suggestion that RCBs were a more valid experimental design than LSs, for both hypothesis testing and precision of estimates. He reached this conclusion using potential outcomes, which he introduced in 1923 as part of his doctoral dissertation (Neyman, 1990), the first place formalizing, explicitly, the notation of potential outcomes for completely randomized (CR) experiments. Neyman (1935) extended this framework in a natural way from CR designs to RCBs and LSs, and calculated the expected mean residual sum of squares and expected mean treatment sum of squares for both.

Neyman (1935) stated that, under the null hypothesis of zero average treatment effects (*Neyman's null hypothesis*), the expected mean residual sum of squares equals the expected mean treatment sum of squares for RCBs, whereas the expected mean residual sum of squares is less than or equal to the expected mean treatment sum of squares for LSs, with equality holding under special cases, such as *Fisher's sharp null hypothesis* of no individual treatment effects. From this comparison of the expected mean residual and treatment sums of squares, Neyman concluded that the standard ANOVA F-test for RCBs was "unbiased", whereas the corresponding test for LSs was "biased", potentially detecting differentiation among the treatments, when none existed on average, more often than desired (i.e., having a higher Type I error than advertised under Neyman's null).

> In the case of the Randomized Blocks the position is somewhat more favourable to the z test [i.e, the F-test], while in the case of the Latin Square this test seems to be biased, showing the tendency to discover differentiation when it does not exist. It is probable that the disturbances mentioned are not important from the point of view of practical applications. (Neyman, 1935, p. 114)

Fisher's fury at Neyman's assertions is evident in his transcribed response:

> Professor R.A. Fisher, in opening the discussion, said he had hoped that Dr. Neyman's paper would be on a subject with which the author was fully acquainted, and on which he could speak with authority .... Since seeing the paper, he had come to the conclusion that Dr. Neyman had been somewhat unwise in his choice of topics. ...Apart from its theoretical defects, Dr. Neyman appears also to have discovered that it [the LS] was, contrary to general belief, a less precise method of experimentation than was supplied by Randomized Blocks, even in those cases in which it had hitherto been regarded as the more precise design. It appeared, too, that they had to thank him, not only for bringing these discoveries to their notice, but also for concealing them from public knowledge until such time as the method should be widely adopted in practice! ...I think it is clear to everyone present that Dr. Neyman has misunderstood the intention ...of the z test and of the Latin Square and other techniques designed to be used with that test. Dr. Neyman thinks that another test would be more important. I am not going to argue that point. It may be that the question which Dr. Neyman thinks should be answered is more important than the one I have proposed and attempted to answer. I suggest that before criticizing previous work it is always wise to give enough study to the subject to understand its purpose. Failing that it is surely quite unusual to claim to understand the purpose of previous work better than its author. (Fisher, 1935, p. 154, 155, 173)

Although Fisher reacted in an intemperate manner, his discussion nevertheless hints at errors in Neyman's calculations. In fact, Fisher was the sole discussant who identified an incorrect equation, (27), in Neyman's appendix:

> Then how had Dr. Neyman been led by his symbolism to deceive himself on so simple a question? ... Equations (13) and (27) of his appendix showed that the quantity which Dr. Neyman had chosen to call σ^2 did not contain the same components of error as those which affected the actual treatment means, or as those which contributed to the estimate of error. (Fisher, 1935, p. 156)

Neyman in fact made a crucial algebraic mistake in his appendix, and his expressions for the expected mean residual sum of squares for both designs are generally

incorrect. We present the correct expressions in Sections 1.2.1 and 1.2.3, and provide an interpretation of these formulae in Section 1.2.5. As we shall see, if one subscribes to Neyman's suggestion that a comparison of expected mean sums of squares determines Type I errors when testing Neyman's null, then the F-test for RCBs is predictably wrong, whereas the F-test for LSs is unpredictably wrong.

However, Neyman's suggestion is generally incorrect. We present in Section 1.3.2 simple examples of LSs for which Neyman's null holds and the expected mean residual sum of squares equals the expected mean treatment sum of squares, yet the Type I error of the F-test is smaller than nominal. Such examples lead to the general result that, for any size RCB or LS, Type I errors are not dictated by a simple comparison of expected sums of squares without further conditions.

A cacophony of commentary on this controversy exists in the literature, and we compiled the most relevant articles in Sections 1.2.2, 1.2.4, and 1.3.1. Our results agree with similar calculations made by Wilk (1955) and Wilk and Kempthorne (1957). A major difference is that we work in a more general setting of Neyman's framework, whereas others, especially Wilk (1955), tend to make further assumptions on the potential outcomes, albeit assumptions possibly justified by applied considerations. Furthermore, although Wilk and Kempthorne (1957) extend Neyman's framework to consider random sampling of rows, columns, and treatment levels from some larger population for LSs, their ultimate suggestion that the expected mean residual sum of squares is larger than the expected mean treatment sum of squares is not generally true. A different parameterization of similar quantities, used in Section 1.2.5, reveals how the inequality could go in either direction.

This controversy had substantial consequences for the subsequent development of statistics for experimental design. As we discuss in Section 1.4.1, deep issues arising from this disagreement led to a shift from *potential outcomes* to additive models for *observed outcomes* in experiments, seriously limiting the scope of inferential tools and reasoning. Our ultimate goal in this historical study is not simply to correct Neyman's algebra. Instead, we wish to highlight the genesis of the current approach to experimental design resulting from this controversy, which is based on linear models and other simple regularity conditions on the potential outcomes that are imprecise without applied contexts.

1.2 Controversial Calculations

1.2.1 Randomized Complete Block Designs: Theory

We first consider RCBs with N blocks, indexed by i, and T treatments, indexed by t, with each block having T experimental units, indexed by $j = 1, \ldots, T$. Treatments are assigned randomly to units in a block, and are applied independently across blocks (Hinkelmann and Kempthorne, 2008, Chap. 9). Although our results hold for general RCB designs, we adopt the same context as Neyman: blocks represent physical blocks of land on a certain field, and we compare agricultural treatments that may affect crop yield, e.g., fertilizers.

We explicitly define treatment indicators $\mathbf{W} = \{W_{ij}(t)\}$ as

$$W_{ij}(t) = \begin{cases} 1 & \text{if unit } j \text{ in block } i \text{ is assigned treatment } t, \\ 0 & \text{otherwise.} \end{cases}$$

Neyman (1935) specified the potential outcomes as

$$x_{ij}(t) = X_{ij}(t) + \epsilon_{ij}(t),$$

where $X_{ij}(t) \in \mathbb{R}$ are unknown constants representing the "mean yield" of unit j in block i under treatment t, and $\epsilon_{ij}(t) \sim [0, \sigma_\epsilon^2]$ are mutually independent and identically distributed (iid) "technical errors", independent of the random variables $\mathbf{W}$. This framework for the potential outcomes, excluding the $\epsilon_{ij}(t)$, is similar to that presented in Neyman's 1923 dissertation (Neyman, 1990).

Neyman (1935, p. 110, 114, 145) stated that technical errors represent inaccuracies in the experimental technique, e.g., inaccuracies in measuring crop yield, and assumed that technical errors are Normal random variables. We find these technical errors rather obscure, but their inclusion does not alter our conclusions. To summarize, in Neyman's specification there are two sources of randomness: the unconfounded assignment mechanism (Rubin, 1990), i.e., the random assignment of treatments to plots specified by the distribution on $\mathbf{W}$, and the technical errors $\epsilon_{ij}(t)$.

Potential outcomes are decomposed by Neyman (1935, p. 111) into

$$x_{ij}(t) = \bar{X}_{\cdot\cdot}(t) + B_i(t) + \eta_{ij}(t) + \epsilon_{ij}(t), \tag{1.2.1}$$

where

$$\bar{X}_{\cdot\cdot}(t) = \frac{1}{NT}\sum_{i=1}^{N}\sum_{j=1}^{T} X_{ij}(t),$$

$$B_i(t) = \bar{X}_{i\cdot}(t) - \bar{X}_{\cdot\cdot}(t),$$

$$\eta_{ij}(t) = X_{ij}(t) - \bar{X}_{i\cdot}(t),$$

with

$$\bar{X}_{i\cdot}(t) = \frac{1}{T}\sum_{j=1}^{T} X_{ij}(t).$$

Neyman describes $B_i(t)$ as a correction for the specific fertility of the i^{th} block, and $\eta_{ij}(t)$ as a correction for fertility variation within the block or, alternatively, the soil error. Hinkelmann and Kempthorne (2008, p. 300) refer to terms such as $\eta_{ij}(t)$ as unit-treatment interactions, but they distinguish between *strict* unit-treatment interactions and block-treatment interactions. For strict unit-treatment interaction, treatment effects depend on the experimental unit, in the sense that for two treatments t, t' and experimental units j, j' in a block i,

$$X_{ij}(t) - X_{ij}(t') \neq X_{ij'}(t) - X_{ij'}(t').$$

Block-treatment interactions are characterized by treatment effects depending on the block, in the sense that for two treatments t, t', experimental units j, j', j'', j''', and blocks i, i',

$$X_{ij}(t) - X_{ij'}(t') \neq X_{i'j''}(t) - X_{i'j'''}(t').$$

As pointed out by a referee, allowing fertility variation to depend on treatment t

was a unique contribution by Neyman and was never recognized in the discussion by Fisher, who focused on his sharp null hypothesis (described next), under which the corrections do not depend on t.

The purpose of the local field experiment, as described by Neyman (1935, p. 111), is to compare the $\bar{X}_{\cdot\cdot}(t)$ for $t = 1, \ldots, T$, each of which represents the average mean yield when one treatment t is applied to all plots in the field, a conceptual experiment. As stated in the discussion, and later by Welch (1937, p. 23), Neyman does not test *Fisher's sharp null hypothesis* of zero individual treatment effects, i.e., (when excluding technical errors),

$$H_0^{\#} : X_{ij}(t) = X_{ij}(t') \; \forall \; i = 1, \ldots, N; \; j = 1, \ldots, T; \; t \neq t'.$$

Instead, Neyman sought to test the more general null hypothesis

$$H_0 : \bar{X}_{\cdot\cdot}(1) = \cdots = \bar{X}_{\cdot\cdot}(T),$$

referred to throughout as *Neyman's null hypothesis*:

> I am considering problems which are important from the point of view of agriculture. And from this viewpoint it is immaterial whether any two varieties react a little differently to the local differences in the soil. What is important is whether on a larger field they are able to give equal or different yields. (Neyman, 1935, p. 173)

If the treatment effects are additive across all units, i.e.,

$$X_{ij}(t) = U_{ij} + \tau(t) \; \forall \; i = 1, \ldots, N; \; j = 1, \ldots, T; \; t = 1, \ldots, T,$$

then testing Neyman's null is equivalent to testing Fisher's sharp null.

The observed yield of the plot assigned treatment t in block i is

$$y_i(t) = \sum_{j=1}^{T} W_{ij}(t) x_{ij}(t),$$

and the observed average yield for all plots assigned treatment t is

$$\bar{y}_{\cdot}(t) = \frac{1}{N} \sum_{i=1}^{N} y_i(t).$$

Neyman (1935, p. 112) noted that an unbiased estimator for the difference between average treatment means, $\bar{X}_{\cdot\cdot}(t) - \bar{X}_{\cdot\cdot}(t')$, is $\bar{y}_{\cdot}(t) - \bar{y}_{\cdot}(t')$, and correctly calculated its sampling variance over its randomization distribution as

$$\mathrm{Var}\{\bar{y}_{\cdot}(t) - \bar{y}_{\cdot}(t')\} = \frac{2\sigma_\epsilon^2}{N} + \frac{\sigma_\eta^2(t) + \sigma_\eta^2(t')}{N} + \frac{2r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')}}{N(T-1)},$$

where

$$\sigma_\eta^2(t) = \frac{1}{NT} \sum_{i=1}^{N} \sum_{j=1}^{T} \eta_{ij}(t)^2,$$

$$r(t,t') = \frac{\sum_{i=1}^{N} \sum_{j=1}^{T} \eta_{ij}(t)\eta_{ij}(t')}{NT\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')}}.$$

Neyman (1935, p. 145) assumed that $\sigma_\eta^2(t)$ and $r(t,t')$ are constant functions of t, t' only to save space and simplify later expressions; this particular set of assumptions appears to have been made purely for mathematical simplicity, and is not driven by any applied considerations, unlike assumptions made by Wilk (1955) and Wilk and Kempthorne (1957) (described in Sections 1.2.2 and 1.2.4).

Neyman then calculated expectations of mean residual sum of squares and mean treatment sum of squares, expressed in our notation as (respectively)

$$S_0^2 = \frac{1}{(N-1)(T-1)} \sum_{i=1}^{N} \sum_{t=1}^{T} \{y_i(t) - \bar{y}_\cdot(t) - \bar{y}_i(\cdot) + \bar{y}_\cdot(\cdot)\}^2,$$

and

$$S_1^2 = \frac{N}{T-1} \sum_{t=1}^{T} \{\bar{y}_\cdot(t) - \bar{y}_\cdot(\cdot)\}^2.$$

As proven in the appendix A.1, the expectations are

$$\begin{aligned}\mathbb{E}(S_0^2) = \sigma_\epsilon^2 &+ \frac{1}{T} \sum_{t=1}^{T} \sigma_\eta^2(t) + \frac{1}{T(T-1)^2} \sum_{t \neq t'} r(t,t') \sqrt{\sigma_\eta^2(t) \sigma_\eta^2(t')} \\ &+ \frac{1}{(N-1)(T-1)} \sum_{i=1}^{N} \sum_{t=1}^{T} \{B_i(t) - \bar{B}_i(\cdot)\}^2,\end{aligned}$$

and

$$\begin{aligned}\mathbb{E}(S_1^2) = \sigma_\epsilon^2 &+ \frac{1}{T} \sum_{t=1}^{T} \sigma_\eta^2(t) + \frac{1}{T(T-1)^2} \sum_{t \neq t'} r(t,t') \sqrt{\sigma_\eta^2(t) \sigma_\eta^2(t')} \\ &+ \frac{N}{T-1} \sum_{t=1}^{T} \{\bar{X}_{\cdot\cdot}(t) - \bar{X}_{\cdot\cdot}(\cdot)\}^2.\end{aligned}$$

Neyman (1935, p. 147-150) correctly calculated the expected mean treatment sum of squares, but made a mistake when calculating the expected mean residual sum of squares. His incorrect expression is equation (27) on page 148. Sukhatme (1935, p. 166), his Ph.D. student at the University of London, incorrectly calculated the expectations for the general case when $\sigma_\eta^2(t)$ and $r(t,t')$ are not constant in t, t', and

the corresponding incorrect expression is his equation (3):

$$\sigma_\epsilon^2 + \frac{1}{T}\sum_{t=1}^{T}\sigma_\eta^2(t) + \frac{1}{T(T-1)^2}\sum_{t\neq t'} r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta(t')}.$$

To see why the last term in $\mathbb{E}(S_0^2)$ is missing in these equations, note that the expression within the brackets of S_0^2 can be written as the sum of the three terms

$$B_i(t) - \bar{B}_i(\cdot),$$

$$\sum_{j=1}^{T} W_{ij}(t)\eta_{ij}(t) - \frac{1}{N}\sum_{i=1}^{N}\sum_{j=1}^{T} W_{ij}(t)\eta_{ij}(t) - \frac{1}{T}\sum_{t=1}^{T}\sum_{j=1}^{T} W_{ij}(t)\eta_{ij}(t) + \frac{1}{NT}\sum_{i=1}^{N}\sum_{t=1}^{T}\sum_{j=1}^{T} W_{ij}(t)\eta_{ij}(t),$$

and

$$\sum_{j=1}^{T} W_{ij}(t)\epsilon_{ij}(t) - \frac{1}{N}\sum_{i=1}^{N}\sum_{j=1}^{T} W_{ij}(t)\epsilon_{ij}(t) - \frac{1}{T}\sum_{t=1}^{T}\sum_{j=1}^{T} W_{ij}(t)\epsilon_{ij}(t) + \frac{1}{NT}\sum_{i=1}^{N}\sum_{t=1}^{T}\sum_{j=1}^{T} W_{ij}(t)\epsilon_{ij}(t).$$

Neyman's equation (17) is missing the first term $B_i(t) - \bar{B}_i(\cdot)$, which is not necessarily equal to zero, and was never explicitly declared to be zero by Neyman.

Consequently, under Neyman's null, the expected mean residual sum of squares is greater than or equal to the expected mean treatment sum of squares, with equality holding if and only if for each block i, $B_i(t)$ is constant across treatments t. Al-

Table 1.1: Table of potential outcomes for a RCB with $\mathbb{E}(S_0^2) > \mathbb{E}(S_1^2)$.

	Treatment 1	Treatment 2
Block 1, Plot 1	10	15
Block 1, Plot 2	10	2
Block 2, Plot 1	20	3
Block 2, Plot 2	30	50

ternatively, equality holds under Fisher's sharp null. If one accepts Neyman's logic regarding "unbiased tests" (discussed in Section 1.3.1), then the correct expressions for the expectations of mean squares suggest that the standard ANOVA F-test for RCBs has a Type I error bounded above by its nominal level.

A simple example makes this concrete. Suppose $N = T = 2$ and $\sigma_\epsilon^2 = 0$, with the potential outcomes in Table 1.1. Note that $\bar{X}_{\cdot\cdot}(1) = \bar{X}_{\cdot\cdot}(2)$, so Neyman's null is satisfied. We calculate $\mathbb{E}(S_0^2) = 215.875,\ \mathbb{E}(S_1^2) = 213.625$, and

$$\mathbb{E}(S_0^2) - \mathbb{E}(S_1^2) = 2.25 = \sum_{i=1}^{2}\sum_{t=1}^{2}\{B_i(t) - \bar{B}_i(\cdot)\}^2.$$

1.2.2 Randomized Complete Block Designs: After the Controversy

Neyman's potential outcomes framework is similar to the "conceptual yield" framework developed by Kempthorne (1952, 1955). Certain features of these two are only cosmetically different: e.g., Kempthorne (1952, p. 137), and later Hinkelmann and Kempthorne (2008, p. 280), represent treatment indicators by δ_{ij}^k (with k denoting treatment level), and potential outcomes as y_{ijk}. As emphasized by a referee, using treatment indicators as random variables provides a mathematical foundation for the

randomization theory of Fisher (1971), connecting potential outcomes with observed responses.

An important difference between Neyman and Kempthorne concerns the notion of technical errors. Hinkelmann and Kempthorne (2008, p. 161) make a distinction between experimental and observational errors, and include separate terms for each, allowing them to depend on treatment. Neyman effectively only considers their sum when defining technical errors, which may be a source of confusion. Of course, Neyman's results were for local field experiments, in which case he might not have considered it necessary to introduce observational errors arising from random sampling of experimental units from some larger population.

Kempthorne (1952) made an interesting comment relating to Fisher's sharp null, Neyman's null, and Neyman's notation for technical errors:

> If the experimenter is interested in the more fundamental research work, Fisher's null hypothesis is more satisfactory, for one should be interested in discovering the fact that treatments have different effects on different plots and in trying to explain why such differences exist. It is only in technological experiments designed to answer specific questions about a particular batch of materials which is later to be used for production of some sort that Neyman's null hypothesis appears satisfactory ... Neyman's hypothesis appears artificial in this respect, that a series of repetitions is envisaged, the experimental conditions remaining the same but the technical errors being different. (Kempthorne, 1952, p. 133)

Furthermore, Kempthorne (1952, p. 145-151) correctly noted (in agreement with our results in Section 1.2.5) that block-treatment interactions must be zero in order for $\mathbb{E}(S_0^2) = \mathbb{E}(S_1^2)$ under Neyman's null, also known as unbiasedness of a design in the Yates (1939) sense. As Kempthorne stated in a later article:

> For the case of randomized blocks it is found that block treatment interactions must be zero in order that the design be unbiased in Yates's sense.

> ... It does not appear to be at all desirable to section the experimental material into ordinary randomized blocks, of ... highly different fertilities (or basal yields) because this procedure is likely to lead to block treatment interactions. (Kempthorne, 1955, p. 964)

Additivity of treatment effects was not invoked by Neyman, and nonadditivity for RCBs was investigated later (Tukey, 1949; Kempthorne, 1955; Wilk, 1955; Mandel, 1961). Perhaps the most substantial work, in the same direction as Neyman, was done by Wilk (1955), who extended the results of Kempthorne (1952, p. 145-151) for RCBs to the case of generalized randomized blocks. Wilk studied randomization moments of mean sums of squares, estimation of various finite-population estimands, and Normal theory approximations for testing Fisher's sharp null and Neyman's null. He also distinguished between experimental error, i.e., the failure of different experimental units treated alike to respond identically, and technical error, or limitations on experimental technique that prevent the exact reproduction of an applied treatment. To us, this use of notation confuses mathematical derivations and practical interpretations of symbols.

More importantly, although Wilk made assumptions on the potential outcomes (consequently not working in our more general setting), he attempted to justify them as physically relevant, as opposed to Neyman, who only made assumptions to facilitate calculations. For example, when translating Wilk's notation into Neyman's, we see that Wilk (1955, p. 72) explicitly considered the physical situation that, if the blocking of experimental units is successful, then the $\eta_{ij}(t) - \bar{\eta}_{ij}(\cdot)$ will be negligible for all i, j, t, whereas block-treatment interactions $B_i(t) - \bar{B}_i(\cdot)$ would be important, in the sense of varying with t. When units in a block are as homogeneous as possible

with respect to background covariates, the assumption of no strict unit-treatment interactions becomes more plausible, similar to the plausibility of zero partial correlation among potential outcomes given all measured covariates. Accordingly, block-treatment interactions become more important. A referee made a similar comment, remarking that for agronomic experiments, it is reasonable to assume that the $\eta_{ij}(t)$ are negligible, whereas in situations such as medical experiments involving human subjects, this may no longer be true.

Wilk's explicit physical consideration is used to justify his assumption (stated without further explanation by Hinkelmann and Kempthorne (2008, p. 301) in their description of the general model for RCBs) that treatments react additively within a block but can react nonadditively from block-to-block: that is,

$$\{X_{ij}(t) - \bar{X}_{ij}(\cdot)\} - \{\bar{X}_{i\cdot}(t) - \bar{X}_{i\cdot}(\cdot)\} = \eta_{ij}(t) - \bar{\eta}_{ij}(\cdot) = 0$$

for all i, j, t, even though

$$B_i(t) - \bar{B}_i(\cdot) \neq 0$$

for at least one pair (i, t). Wilk (1955, p. 73) then stated that, if

$$\eta_{ij}(t) - \bar{\eta}_{ij}(\cdot) \neq 0$$

for at least one triple (i, j, t), then the expected mean treatment sum of squares is not equal to the expected mean residual sum of squares under Neyman's null. Hinkelmann and Kempthorne (2008, p. 301), when summarizing Wilk's work, noted that the expected mean residual sum of squares for RCB designs contains the interaction

between blocking and treatment factors, similar to our result.

1.2.3 Latin Square Designs: Theory

It was in his treatment of LSs that Neyman's error substantially changes conclusions. We consider $T \times T$ LSs with rows and columns denoting levels of two blocking factors, e.g., north-south and east-west. Our treatment indicators are

$$W_{ij}(t) = \begin{cases} 1 & \text{if the unit in row } i, \text{ column } j, \text{ is assigned treatment } t, \\ 0 & \text{otherwise.} \end{cases}$$

Neyman specified the potential outcomes as

$$x_{ij}(t) = X_{ij}(t) + \epsilon_{ij}(t),$$

with $X_{ij}(t) \in \mathbb{R}$ unknown constants representing the "mean yield" of the unit in cell (i, j) under treatment t, and $\epsilon_{ij}(t) \sim [0, \sigma_\epsilon^2]$ technical errors that are iid and independent of $\mathbf{W}$. Potential outcomes were then decomposed into

$$x_{ij}(t) = \bar{X}_{\cdot\cdot}(t) + R_i(t) + C_j(t) + \eta_{ij}(t) + \epsilon_{ij}(t), \tag{1.2.2}$$

where

$$R_i(t) = \bar{X}_{i\cdot}(t) - \bar{X}_{\cdot\cdot}(t),$$

$$C_j(t) = \bar{X}_{\cdot j}(t) - \bar{X}_{\cdot\cdot}(t),$$

$$\eta_{ij}(t) = X_{ij}(t) - \bar{X}_{i\cdot}(t) - \bar{X}_{\cdot j}(t) + \bar{X}_{\cdot\cdot}(t).$$

Similar to RCBs, Neyman described $R_i(t)$ and $C_j(t)$ as corrections for specific soil fertility of the i^{th} row and j^{th} column, respectively, and $\eta_{ij}(t)$ as the soil error for plot (i, j) under treatment t.

We define $\bar{x}^o_{\cdot\cdot}(t)$ as the observed average yield for plots assigned treatment t,

$$\bar{x}^o_{\cdot\cdot}(t) = \frac{1}{T}\sum_{i=1}^{T}\sum_{j=1}^{T} W_{ij}(t)x_{ij}(t).$$

Neyman (1935) correctly noted that $\mathbb{E}\{\bar{x}^o_{\cdot\cdot}(t) - \bar{x}^o_{\cdot\cdot}(t')\} = \bar{X}_{\cdot\cdot}(t) - \bar{X}_{\cdot\cdot}(t')$, and that

$$\mathrm{Var}\{\bar{x}^o_{\cdot\cdot}(t) - \bar{x}^o_{\cdot\cdot}(t')\} = \frac{2\sigma^2_\epsilon}{T} + \frac{\sigma^2_\eta(t) + \sigma^2_\eta(t')}{T-1} + \frac{2r(t,t')\sqrt{\sigma^2_\eta(t)\sigma^2_\eta(t')}}{(T-1)^2}.$$

Neyman then calculated the expected mean sums of squares. The mean residual and treatment sums of squares are defined as (respectively)

$$S^2_0 = \frac{1}{(T-1)(T-2)}\sum_{i=1}^{T}\sum_{j=1}^{T}\left\{y_{ij} - \bar{y}_{i\cdot} - \bar{y}_{\cdot j} - \sum_{t=1}^{T} W_{ij}(t)\bar{x}^o_{\cdot\cdot}(t) + 2\bar{y}_{\cdot\cdot}\right\}^2,$$

and

$$S^2_1 = \frac{T}{T-1}\sum_{t=1}^{T}\{\bar{x}^o_{\cdot\cdot}(t) - \bar{y}_{\cdot\cdot}\}^2,$$

with $y_{ij} = \sum_{t=1}^{T} W_{ij}(t)x_{ij}(t)$ the observed response of cell (i, j), and

$$\bar{y}_{i\cdot} = \frac{1}{T}\sum_{j=1}^{T} y_{ij}, \quad \bar{y}_{\cdot j} = \frac{1}{T}\sum_{i=1}^{T} y_{ij}, \quad \bar{y}_{\cdot\cdot} = \frac{1}{T}\sum_{j=1}^{T}\bar{y}_{\cdot j} = \frac{1}{T}\sum_{i=1}^{T}\bar{y}_{i\cdot}$$

We prove in the appendix A.2 that the correct expectations are

$$\mathbb{E}(S_0^2) = \sigma_\epsilon^2 + \frac{T-2}{(T-1)^2}\sum_{t=1}^{T}\sigma_\eta^2(t) + \frac{2}{(T-1)^3}\sum_{t\neq t'} r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')} + \frac{1}{T(T-1)^2}\sum_{i=1}^{T}\sum_{j=1}^{T}\sum_{t=1}^{T}[\{R_i(t) - \bar{R}_i(\cdot)\}^2 + \{C_j(t) - \bar{C}_j(\cdot)\}^2],$$

and

$$\mathbb{E}(S_1^2) = \sigma_\epsilon^2 + \frac{1}{T-1}\sum_{t=1}^{T}\sigma_\eta^2(t) + \frac{1}{(T-1)^3}\sum_{t\neq t'} r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')} + \frac{T}{T-1}\sum_{t=1}^{T}\{\bar{X}_{\cdot\cdot}(t) - \bar{X}_{\cdot\cdot}(\cdot)\}^2.$$

Neyman (1935, p. 152) made a similar mistake as he did for RCBs, excluding

$$R_i(t) + C_j(t) - \bar{R}_i(\cdot) - \bar{C}_j(\cdot)$$

in a simplified expression for the term inside the brackets of S_0^2 in his equation (50). In effect, Neyman once again excluded corrections for soil fertility, as it is not necessarily true (nor stated explicitly) that $R_i(t)$ is constant in t for all rows i and that $C_j(t)$ is constant in t for all columns j. Sukhatme (1935, p. 167) made a similar mistake for the case when $\sigma_\eta^2(t)$ and $r(t,t')$ are not constant in t, t'.

After incorrectly calculating the expected mean residual sum of squares, Neyman stated that the expected mean residual sum of squares was less than or equal to the expected mean treatment sum of squares under Neyman's null (Neyman, 1935, p. 154), with equality only under special cases, such as Fisher's sharp null. Based on

this observation, Neyman conjectured that the standard ANOVA F-test for LSs is potentially invalid in the sense of having a higher Type I error than nominal, i.e., rejecting more often than desired under Neyman's null.

However, the expected mean residual sum of squares is not necessarily less than the expected mean treatment sum of squares under Neyman's null. In fact, the inequality could go in either direction. We describe in Section 1.2.5 how the inequality depends on interactions between row/column blocking factors and the treatment.

Two examples of LSs with $T = 3$, $\sigma_\epsilon^2 = 0$, and $\bar{X}_{\cdot\cdot}(1) = \bar{X}_{\cdot\cdot}(2) = \bar{X}_{\cdot\cdot}(3)$ (i.e., Neyman's null) demonstrate this fact. In Tables 1.2 and 1.3, each unit's potential outcomes are represented by an ordered triple, with the t^{th} coordinate denoting the potential outcome under treatment t. For Table 1.2, $\mathbb{E}(S_0^2) = 252.07,\ \mathbb{E}(S_1^2) = 172.38$. From our formulae,

$$\begin{aligned}\mathbb{E}(S_0^2) - \mathbb{E}(S_1^2) = & -\frac{1}{(T-1)^2}\sum_{t=1}^{T}\sigma_\eta^2(t) + \frac{1}{(T-1)^3}\sum_{t\neq t'} r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')} \\ & + \frac{1}{T(T-1)^2}\sum_{i=1}^{T}\sum_{j=1}^{T}\sum_{t=1}^{T}[\{R_i(t) - \bar{R}_i(\cdot)\}^2 + \{C_j(t) - \bar{C}_j(\cdot)\}^2].\end{aligned}$$

We verify by explicit randomization that the discrepancy $\mathbb{E}(S_0^2) - \mathbb{E}(S_1^2) = 79.69$ equals this expression, so that this is one LS for which the expected mean residual sum of squares is greater than the expected mean treatment sum of squares. The inequality is in the other direction for Table 1.3, with $\mathbb{E}(S_0^2) = 4.96,\ \mathbb{E}(S_1^2) = 6.77$.

Table 1.2: Table of potential outcomes for a LS with $\mathbb{E}(S_0^2) > \mathbb{E}(S_1^2)$.

	Column 1	Column 2	Column 3
Row 1	$(3, 10, 15)$	$(50, 30, 13)$	$(20, 20, 40)$
Row 2	$(10, 13, 50)$	$(20, 40, 3)$	$(30, 15, 20)$
Row 3	$(13, 3, 20)$	$(15, 20, 10)$	$(40, 50, 30)$

Table 1.3: Table of potential outcomes for a LS with $\mathbb{E}(S_0^2) < \mathbb{E}(S_1^2)$.

	Column 1	Column 2	Column 3
Row 1	$(7, 4, 8)$	$(5, 9, 4)$	$(6, 6, 5)$
Row 2	$(8, 5, 6)$	$(3, 3, 3)$	$(2, 2, 7)$
Row 3	$(1, 8, 2)$	$(4, 7, 9)$	$(9, 1, 1)$

1.2.4 Latin Square Designs: After the Controversy

As with RCBs, no additivity assumption is made on the potential outcomes for LSs. Nonadditivity for LSs has been further studied in the literature (Gourlay, 1955b; Tukey, 1955; Rojas, 1973). Kempthorne recognized the issue of interactions between row/column blocking factors and the treatment factor in a LS (discussed in the next section):

> It is clear that, if there are row-treatment or column-treatment interactions, these will enter into the error mean square but not into the treatment mean square. The situation is entirely analogous to that of randomized blocks in that block-treatment interactions enter the error mean square but not the treatment mean square. (Kempthorne, 1952, p. 195)

Kempthorne (1952, p. 204) continued by noting a defect of large LSs, namely that there are more opportunities for row/column interactions with treatments.

A substantial investigation in the spirit of Neyman was perfomed by Wilk and Kempthorne (1957), and is briefly summarized by Hinkelmann and Kempthorne (2008, p. 387). Wilk and Kempthorne (1957, p. 224) adopt the same specification of potential outcomes as Neyman (1935), allowing technical errors to differ based on

treatment level k:

$$y_{ijk} = Y_{ijk} + \epsilon_{ijk}.$$

One difference that makes the conceptual yield framework of Wilk and Kempthorne more general is that they consider randomly sampling rows, columns, and treatments from some larger population. In any case, Wilk and Kempthorne (1957, p. 227) reach the reverse conclusion as Neyman, stating that, usually, the expected mean residual sum of squares is larger than the expected mean treatment sum of squares. Wilk and Kempthorne (1957, p. 227) explain this difference, and the fact that Neyman did not recognize interactions between row/column blocking factors and the treatments, by noting that Neyman (1935, p. 145) made additional homogeneity assumptions. However, Neyman's assumptions were invoked solely to facilitate calculations, and had no physical justifications.

Our results are in agreement with a summary of their work in Table 3 from (Wilk and Kempthorne, 1957, p. 226). Thus, it appears that Wilk and Kempthorne do not seriously consider the possibility that the inequality could go in the direction Neyman claimed. In fact, Hinkelmann and Kempthorne (2008, p. 387), when summarizing this paper, explicitly state that the expected mean residual sum of squares is larger than the expected mean treatment sum of squares under Neyman's null. A possible explanation can be found in the sixth remark on page 227, where Wilk and Kempthorne discuss how the standard approach to designing LSs may likely result in interactions of row/column blocking factors with treatments. As explained in our next section, the magnitudes of these interactions ultimately drive the direction of the inequality.

Cox (1958a) built on the work of Wilk and Kempthorne, and provided a rather unique viewpoint on this entire problem. After first summarizing Wilk and Kempthorne's results by stating that it is usually the case that the expected mean residual sum of squares is larger than the expected mean treatment sum of squares, Cox then considered the practical importance of this difference of expectations, which he correctly recognized as being related to interactions between the treatment and blocking factors. Cox (1958a, p. 73) raised the thought-provoking question of whether, for a LS, the practical scientific interest of the null

$$H_0 : \mathbb{E}(S_0^2) = \mathbb{E}(S_1^2)$$

is comparable to, or greater than, Neyman's null, especially when the difference between these expected mean sums of squares is considered important. He concluded that testing Neyman's null when there is no unit-treatment additivity does not seem to be helpful:

> ... if substantial variations in treatment effect from unit to unit do occur, one's understanding of the experimental situation will be very incomplete until the basis of this variation is discovered and any extension of the conclusions to a general set of experimental units will be hazardous. The mean treatment effect, averaged over all units in the experiment, or over the finite population of units from which they are randomly drawn, may in such cases not be too helpful. Particularly if appreciable systematic treatment-unit interactions are suspected, the experiment should be set out so these may be detected and explained. (Cox, 1958a, p. 73)

Cox (2012, p. 3) later argued that when this more realistic null is formulated, the biases described earlier disappear, and so do issues surrounding the LS. A related point for the LS design noted by Cox is the marginalization principle, in which models

having nonzero interactions and zero main effects are not considered sensible (similar to the effect heredity principle (Wu and Hamada, 2009, p. 173)). Box (1984), when commenting on Cox (1984), provided an opposing view that makes such a principle context-dependent.

1.2.5 Block-Treatment Interactions and Expected Sums of Squares

Neyman excluded the following (respective) terms in $\mathbb{E}(S_0^2)$ for RCBs and LSs:

$$\frac{1}{(N-1)(T-1)} \sum_{i=1}^{N} \sum_{t=1}^{T} \{B_i(t) - \bar{B}_i(\cdot)\}^2,$$

$$\frac{1}{(T-1)^2} \sum_{i=1}^{T} \sum_{t=1}^{T} \{R_i(t) - \bar{R}_i(\cdot)\}^2 + \frac{1}{(T-1)^2} \sum_{j=1}^{T} \sum_{t=1}^{T} \{C_j(t) - \bar{C}_j(\cdot)\}^2.$$

In each, we are adding squared differences between the fertility correction for a specific combination of block and treatment levels, and the average (over treatments) fertility correction for the same block level. For the LS, this is decomposed as a sum over the row and a sum over the column blocking factors.

Formally, these terms gauge whether, for each level of a blocking factor, the fertility corrections are constant over the treatments, and represent interactions between blocking factors and treatments. For RCBs, we have

$$B_i(t) - \bar{B}_i(\cdot) = \{\bar{X}_{i\cdot}(t) - \bar{X}_{i\cdot}(\cdot)\} - \{\bar{X}_{\cdot\cdot}(t) - \bar{X}_{\cdot\cdot}(\cdot)\},$$

which is the interaction between the i^{th} block and the t^{th} treatment in terms of

potential outcomes. Similarly, we have for LSs that

$$R_i(t) - \bar{R}_i(\cdot) = \{\bar{X}_{i\cdot}(t) - \bar{X}_{i\cdot}(\cdot)\} - \{\bar{X}_{\cdot\cdot}(t) - \bar{X}_{\cdot\cdot}(\cdot)\},$$

$$C_j(t) - \bar{C}_j(\cdot) = \{\bar{X}_{\cdot j}(t) - \bar{X}_{\cdot j}(\cdot)\} - \{\bar{X}_{\cdot\cdot}(t) - \bar{X}_{\cdot\cdot}(\cdot)\},$$

which are the interactions between the i^{th} row and t^{th} treatment, and the j^{th} column and the t^{th} treatment, respectively, in terms of potential outcomes.

Intuitively, these interactions, which are functions of potential outcomes, should reside within the expectation of the mean residual sum of squares. Without invoking additivity on the potential outcomes, these interactions are not necessarily zero, and because we lack replications within blocks for either RCB or LS designs, we cannot form an interaction sum of squares from the observed data, so that the potential outcome interactions will instead be included in the expectation of the mean residual sum of squares (Fisher, 1971, Chap. IV, V). In contrast, for randomized block designs that include replications within each block, this interaction term is no longer present in the expected mean residual sum of squares.

To better understand the expected mean sums of squares for LSs, consider their difference under Neyman's simplifying assumption that $\sigma^2_\eta(t)$ and $r(t, t')$ are constant, so that $\sigma^2_\eta(t) = \sigma^2_\eta$, and $r(t, t') = r$ for all treatments t, t'. Then the difference between $\mathbb{E}(S_0^2)$ and $\mathbb{E}(S_1^2)$ under Neyman's null is

$$\sum_{i=1}^{T}\sum_{t=1}^{T}\{R_i(t) - \bar{R}_i(\cdot)\}^2 + \sum_{j=1}^{T}\sum_{t=1}^{T}\{C_j(t) - \bar{C}_j(\cdot)\}^2 - T\sigma^2_\eta(1-r),$$

and this expression, in some sense, measures the difference between row/column in-

teractions with treatment, and the variance of the potential outcome residual terms (scaled by the number of treatments, T, times one minus the correlation between potential outcome residual terms for different pairs of treatments). Note that $0 \leq 1 - r \leq 2$, so $0 \leq T\sigma_\eta^2(1-r) \leq 2T\sigma_\eta^2$.

To interpret the difference in expectations for the general case, first note that

$$\sum_{i=1}^{T}\sum_{j=1}^{T}\bar{\eta}_{ij}(\cdot)^2 \geq 0 \Rightarrow \sum_{t=1}^{T}\sigma_\eta^2(t) \geq -\sum_{t\neq t'} r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')}.$$

As such, $\mathbb{E}(S_0^2) - \mathbb{E}(S_1^2)$ under Neyman's null is bounded from below by

$$\frac{1}{(T-1)^2}\sum_{i=1}^{T}\sum_{t=1}^{T}\{R_i(t)-\bar{R}_i(\cdot)\}^2+\frac{1}{(T-1)^2}\sum_{j=1}^{T}\sum_{t=1}^{T}\{C_j(t)-\bar{C}_j(\cdot)\}^2-\frac{T}{(T-1)^3}\sum_{t=1}^{T}\sigma_\eta^2(t),$$

so that, if

$$\sum_{i=1}^{T}\sum_{t=1}^{T}\{R_i(t)-\bar{R}_i(\cdot)\}^2+\sum_{j=1}^{T}\sum_{t=1}^{T}\{C_j(t)-\bar{C}_j(\cdot)\}^2-\frac{T}{T-1}\sum_{t=1}^{T}\sigma_\eta^2(t) \geq 0,$$

then $\mathbb{E}(S_0^2) \geq \mathbb{E}(S_1^2)$. Even in the most general case for LSs, $\mathbb{E}(S_0^2) - \mathbb{E}(S_1^2)$ can still be interpreted as a comparison between row/column interactions with treatment and the (scaled) sum of variances of residual potential outcomes $\eta_{ij}(t)$.

In the context of an agricultural experiment, we obtain a more meaningful interpretation for this difference. Latin squares are implemented to block on fertility gradients in two directions (Neyman, 1935; Fisher, 1971, Chap. V; Hinkelmann and Kempthorne, 2008, Chap. 10). If the variability of specific soil fertility corrections across rows and columns (i.e., interactions between rows/columns and treatments)

are substantially larger than the residual variability of the potential outcomes (i.e., the variability of the $\eta_{ij}(t)$), then $\mathbb{E}(S_0^2) - \mathbb{E}(S_1^2)$ is larger than zero. An example was given in Table 1.2, where

$$\sum_{i=1}^{T}\sum_{t=1}^{T}\{R_i(t) - \bar{R}_i(\cdot)\}^2 + \sum_{j=1}^{T}\sum_{t=1}^{T}\{C_j(t) - \bar{C}_j(\cdot)\}^2 = 569.93,$$

$$-\sum_{t=1}^{T}\sigma_\eta^2(t) = -313.56,$$

$$\frac{1}{T-1}\sum_{t\neq t'} r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')} = 62.41.$$

The interaction is nearly twice the variability of the residual potential outcomes, and so the difference $\mathbb{E}(S_0^2) - \mathbb{E}(S_1^2)$ is greater than zero. For Table 1.3,

$$\sum_{i=1}^{T}\sum_{t=1}^{T}\{R_i(t) - \bar{R}_i(\cdot)\}^2 + \sum_{j=1}^{T}\sum_{t=1}^{T}\{C_j(t) - \bar{C}_j(\cdot)\}^2 = 9.48,$$

$$-\sum_{t=1}^{T}\sigma_\eta^2(t) = -14.59,$$

$$\frac{1}{T-1}\sum_{t\neq t'} r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')} = -2.11,$$

and the variance of the residuals completely dominates the interaction.

Hence, $\mathbb{E}(S_0^2) > \mathbb{E}(S_1^2)$ in the presence of a strong fertility gradient, with the interaction between row/column blocking factors and treatment greater than the variance of the residual potential outcomes or, alternatively, when the unit-treatment interactions are negligible. Similarly, $\mathbb{E}(S_0^2) < \mathbb{E}(S_1^2)$ in cases where no strong interaction exists between row/column blocking factors and the treatment when compared to

the variability of the residual potential outcomes or, alternatively when the unit-treatment interactions are substantial. It is important to recognize that such important interactions can never be assessed without replication, which is not available in the original LS design.

1.3 Controversial Connections

1.3.1 Connecting Expected Mean Sums of Squares with Type I Error

Neyman (1935) calculated expectations of mean sums of squares to argue that the standard ANOVA F-test for RCB designs is valid and the test for LS designs is invalid when testing Neyman's null: a test was said to be "unbiased" if $\mathbb{E}(S_0^2) = \mathbb{E}(S_1^2)$ under Neyman's null (Neyman, 1935, p. 144). The reasoning behind this definition is not discussed at all, and, given our current understanding of hypothesis testing, seems somewhat crude. After all, to determine whether a particular testing procedure is "biased", one typically calculates the probability of rejecting a true null hypothesis, which generally depends on the test statistic's distribution, not just its expectation.

To better understand the logic potentially driving Neyman's reasoning, it is useful to review the testing of Fisher's sharp null. A randomization test that uses any *a priori* defined test statistic automatically yields the correct Type I error under Fisher's sharp null and regularity conditions on the potential outcomes and number of randomizations. Furthermore, when using the statistic $F = S_1^2/S_0^2$, this randomization distribution is well-approximated by the F-distribution, for both RCB and LS

designs. Welch (1937) calculated the first two moments of

$$\frac{df_1 S_1^2}{df_1 S_1^2 + df_0 S_0^2} = \frac{df_1 F}{df_1 F + df_0}, \tag{1.3.1}$$

where df_1 denotes the degrees of freedom for treatment sum of squares, and df_0 the degrees of freedom for residual sum of squares. Pitman (1938) calculated the first four moments of this statistic. For both RCB and LS designs, $df_1 S_1^2 + df_0 S_0^2$ remains constant over the randomizations under Fisher's sharp null, making calculation of the moments of (1.3.1) much easier than of F itself. Furthermore, under regularity conditions on the potential outcomes, it was shown that these moments are approximately equal to the corresponding moments of a Beta distribution. In this respect, the standard ANOVA F-test that uses rejection cutoffs based on the F-distribution has approximately the correct Type I error, and the F-distribution can be viewed as a simple approximation to the randomization distribution of the F-test statistic when testing Fisher's sharp null (Kempthorne, 1952, p. 172, 193). Indeed, as stated by Wilk (1955, p. 77), the amount of computation to perform a randomization test could be prohibitive, and statisticians had little recourse except to use such approximations. Kempthorne made a similar remark:

> It should be realized that the analysis of variance test with the F distribution has a fair basis apart from normal law theory and is probably in most cases a good approximation to the randomization analysis of variance test, which is a nonparametric test. (Kempthorne, 1955, p. 966)

Kempthorne earlier stated that for LSs:

> The randomization test for the Latin Square or for any randomized design is entirely valid in the sense of controlling Type I errors, but the approximation to this test by the F-distribution when there is non-additivity is apparently completely unknown. (Kempthorne, 1955, p. 965)

As Neyman did not invoke additivity or any other regularity conditions on the potential outcomes, the reasoning outlined in the previous paragraph that establishes the F-distribution as an approximation to the true distribution of the F-test statistic is no longer valid when testing Neyman's null: e.g., $df_1 S_1^2 + df_0 S_0^2$ is generally no longer constant over the randomizations, and calculating moments of equation (1.3.1) generally becomes very difficult. Wilk (1955, p. 79) realized this, remarking that the standard ANOVA F-test for testing Neyman's null in RCBs depends on the assumption that block-treatment interactions are zero. Wilk and Kempthorne (1957, p. 228) also stated that the effect of nonadditivity on the Type I error of the standard ANOVA F-test for a LS is unknown.

Bearing these facts in mind, a comparison of expected mean residual and treatment sums of squares could be viewed as a crude way of assessing whether the Type I error is correct when testing Neyman's null using the standard ANOVA F-test. Neyman (1935) himself may have realized this:

> ... in the case of the Randomized Blocks the z test may be considered as unbiased in the sense that the expectations of S_0^2 and S_1^2 have a common value ... On the other hand, by the arrangement in Latin Square the expectation of S_1^2 is equal to $\frac{1}{2}n'\sigma_d^2$, while that of S_0^2 is generally smaller. This suggests, although it does not prove, that by the Latin Square arrangement the z test may have the tendency to detect differentiation when it does not exist. (Neyman, 1935, p. 144)

After calculating expected mean sums of squares for RCBs, Neyman states that:

> If there is no differentiation among the $X_{\cdot\cdot}(k)$, then $\mathbb{E}(S_1^2) = \mathbb{E}(S_0^2)$, and we see that the test of significance usually applied is unbiased in the sense that if there is no differentiation, then the values of S_1^2 and S_0^2 must be approximately equal. This, of course, does not prove the validity of Fisher's z test. (Neyman, 1935, p. 150)

Furthermore, Neyman states that for LSs:

> We conclude, therefore, that at present there is no theoretical justification for the belief that the z test is valid in the case of the arrangement by the Latin Square: not only is there the difficulty connected with the non-normality of the distribution of the η's, but also the functions which are usually considered as unbiased estimates of the same variance have generally different expectations. This may (though not necessarily so) cause a tendency to state significant differentiation when this, in fact, does not exist. ... These, of course, are purely theoretical conclusions, and I am personally inclined to think that from the practical point of view the existing bias will prove to be negligible. (Neyman, 1935, p. 154)

This same consideration of expected mean sums of squares for hypothesis testing continues in the present literature on experimental design.

> It is the form of the expected mean squares, $\mathbb{E}[\text{MS}(i)]$, which determines, for example, how tests of hypotheses are performed and how error variances are estimated. (Hinkelmann and Kempthorne, 2008, p. 37)

Also:

> In this case, MS(E) is on average larger than MS(T) under the hypothesis of no treatment effects and hence the usual F-test will lead to fewer significant results. In this case the LSD is not an unbiased design. (Hinkelmann and Kempthorne, 2008, p. 387)

It is interesting to note that the specific justification for this last statement was never made, nor was any attempt made to calculate explicitly the Type I error. Even more interesting is how these statements contradict Kempthorne's earlier position on the connection between expected mean sums of squares and hypothesis testing (e.g., as given by Kempthorne (1952, p. 149)). For example:

> To establish the property of unbiasedness for this design it is ... necessary to show that the expectation over randomizations of the error mean square resulting from this model is equal to the mean square among all observations in the absence of treatment effects. ... it should perhaps be noted that this property has no intrinsic relation to the concept of unbiasedness of a test. (Kempthorne, 1955, p. 956)

Wilk and Kempthorne (1957) hold this same position, stating that:

> We accept the view that tests of significance are evaluatory procedures leading to assessments of strength of evidence against particular hypotheses, while tests of hypotheses are decision devices. We are here concerned with the former, and in this connection it should be noted that (a) the expectations of mean squares are in some degree irrelevant to the exact (permutation) test of significance of the null hypothesis that the treatments are identical. (Wilk and Kempthorne, 1957, p. 228)

1.3.2 Concrete Calculations

From Section 1.2.1, the F-test for RCBs is generally biased in one direction under Neyman's conception of an unbiased test, potentially leading to fewer rejections under Neyman's null. Furthermore, because we do not make any assumptions about the difference between the interactions of rows/columns with treatment and the residual variances in Section 1.2.3, we actually cannot claim that the F-test for LSs is biased in any one direction. A more rigorous justification for the "unbiasedness" of the F-test for either design would compare the actual distribution of the F-test statistic to the associated F-distribution. By determining whether the distribution of $F = S_1^2/S_0^2$ is adequately approximated by the F-distribution under Neyman's null, one would be able to conclude whether the Type I error is approximately as advertised.

We performed this comparison for various RCBs and LSs, and observed that Neyman's definition of unbiased tests fails. In particular, we can generate infinitely many RCBs and LSs such that (1) Neyman's null holds, (2) there is no interaction between blocking factor(s) and treatment, (3) the expected mean residual sum of squares equals the expected mean treatment sum of squares, and yet there is zero probability of rejecting Neyman's null when the rejection rule is based on a comparison

Table 1.4: Table of potential outcomes for a 4×4 LS, with $\mathbb{E}(S_0^2) = \mathbb{E}(S_1^2)$.

	Column 1	Column 2	Column 3	Column 4
Row 1	$(1,1,1,1)$	$(0,0,0,0)$	$(0,0,0,0)$	$(0,0,0,0)$
Row 2	$(0,0,0,0)$	$(1,1,1,1)$	$(0,0,0,0)$	$(0,0,0,0)$
Row 3	$(0,0,0,0)$	$(0,0,0,0)$	$(0,0,0,0)$	$(0,0,0,0)$
Row 4	$(0,0,0,0)$	$(0,0,0,0)$	$(0,0,0,0)$	$(0,0,0,0)$

of the observed value of S_1^2/S_0^2 with $\alpha = 0.05$ cutoffs used in the standard ANOVA F-test.

For simplicity, consider the case with no technical errors. One simple example of a 4×4 LS, with $\sigma_\eta^2(t)$, $r(t,t')$ constant, $\mathbb{E}(S_0^2) = \mathbb{E}(S_1^2)$, and no interactions between row/column blocking factors and the treatment, is presented in Table 1.4. Now $F_{3,6,0.95} = 4.76$ and, as we have all potential outcomes, we can calculate the probability that $S_1^2 > kS_0^2$ for any positive number k over the distribution of S_1^2 and S_0^2. These probabilities are given in the left of Figure 1.1, which also displays probabilities that $F_{3,6} > k$; probabilities from the randomization distribution of S_1^2/S_0^2 are plotted as dots, and probabilities for the $F_{3,6}$ distribution as dashes. A horizontal line at 0.05 and a vertical line at 4.76 were drawn to illustrate conclusions obtained at the 0.05 significance level. The probability of rejecting Neyman's null when using the standard ANOVA F-test is zero.

The crucial factor here is the structure of the potential outcomes. Fisher's sharp null holds, so the total sum of squares, and the sum of squares for row and column blocking factors, remain constant over the randomization. Furthermore, the treatment sum of squares takes only two values, corresponding to whether cells $(1,1)$ and $(2,2)$ receive the same treatment or not, and similarly the residual sum of squares takes only two values. Hence, the F-test statistic takes only two possible values, so

that cutoffs given by consideration of the F-distribution will not yield approximately correct Type I errors for testing Neyman's null.

Inclusion of technical errors does not change our general conclusion. Suppose technical errors are Normally distributed with $\sigma_\epsilon = 0.01$. The corresponding figure for the LS in Table 1.4 is displayed in the right of Figure 1.1. We generated this figure by simulation: we first drew $\epsilon_{ij}(t)$, then performed the randomizations to generate the distribution of S_1^2 and S_0^2 for that specific draw of technical errors, and finally repeated this process 2000 times to estimate the probabilities.

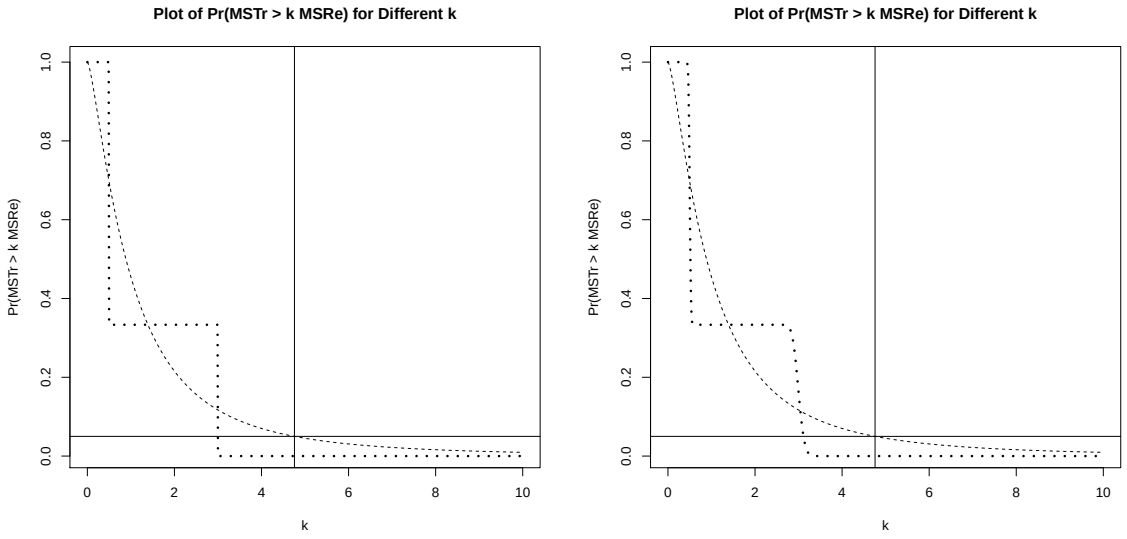

Figure 1.1: Comparison of the distributions of S_1^2/S_0^2 and $F_{3,6}$ for Table 1.4; the distribution of S_1^2/S_0^2 is represented by dots, and that of $F_{3,6}$ by dashes. The figure on the left is for the case with no technical errors, and the figure on the right is for technical errors with $\sigma_\epsilon = 0.01$.

1.4 Controversial Consequences and Conclusions

1.4.1 Consequences

The most immediate consequence of this entire controversy was the resulting hostile relationship between Neyman and Fisher for essentially the remainder of their careers, with each seeking to undermine the other. For example, Neyman was slightly critical in a discussion of a paper presented by Yates (1935) on factorial designs. Box (1978, p. 265) claimed that Neyman wanted to demonstrate his superiority by finding flaws in Fisher's work at this meeting. Reid (1982, p. 126) described an interesting encounter between Neyman and Fisher, taking place in Neyman's room at University College London one week after this discussion. Fisher demanded that Neyman only use Fisher's books when lecturing on statistics at the university. When Neyman refused to do so, Fisher openly declared that he would oppose Neyman in all his capacities, and banged the door when he left the room.

These skirmishes continued for some time (Reid, 1982, p. 143, 169, 183-184, 223-226, 256-257). Neyman appears to have attempted some type of reconciliation, inviting Fisher to lecture at Berkeley (Reid, 1982, p. 222), and generally became more conciliatory toward Fisher and his contributions to statistics (Neyman, 1976; Reid, 1982, p. 45). In any case, these passages suggest an indirect consequence of this controversy: Neyman's decision to depart for America, where he created a world-class center for statistics at the University of California Berkeley (Reid, 1982, p. 239), established a prominent series of symposia (Reid, 1982, p. 197-198), and helped to nurture, through his leadership, the American Statistical Association and Institute of

Mathematical Statistics (Reid, 1982, p. 218).

Fienberg and Tanur (1996) suggest that this break in the professional relationship between Neyman and Fisher may have led to a sharper division between the fields of sample surveys and experimental design:

> Because of the bitterness that grew out of this dispute ... Fisher and Neyman were never able to bring their ideas together and benefit from the fruitful interaction that would likely have occurred had they done so. And in the aftermath, Neyman staked out intellectual responsibility for sampling while Fisher did the same for experimentation. It was in part because of this rift between Fisher and Neyman that the fields of sample surveys and experimentation drifted apart. (Fienberg and Tanur, 1996, p. 238)

Cox (2012) makes the interesting remark that more effort was devoted to issues in randomization following this controversy:

> The general issues of the role of randomization were further discussed in the next few years, mostly in *Biometrika*, with contributions from Student, Yates, Neyman and Pearson, and Jeffreys. With the exception of Student's contribution, which emphasized the role of randomization in escaping biases arising from personal judgement, the discussion focused largely on error estimation. (Cox, 2012, p. 3)

Another consequence was undue emphasis on linear models for analysis of experimental data. As stated by Gourlay (1955a, p. 228), Neyman's work in 1935 led to increased attention on models (for observed data) that formed the basis of statistical analyses such as ANOVA. Eisenhart (1947), for example, explicitly laid out the four standard assumptions used to justify ANOVA, and noted the importance of additivity. Immediately following this article, Cochan (1947) explored the consequences for an analysis when additivity (and the other assumptions) were not satisfied, and Bartlett (1947) discussed various transformations of the data that make additivity more plausible for ANOVA.

Accordingly, past and present books on experimental design tend to invoke additive models when testing Neyman's null using the standard ANOVA F-test, an assumption that automatically yields a test of Fisher's sharp null (Kempthorne, 1952, Chap. 8, 9, 10; Hinkelmann and Kempthorne, 2008, Chap. 9, 10). When additivity is believed not to hold, one is generally advised to search for a transformation that yields an additive structure on the potential outcomes. For example, Wilk and Kempthorne (1957, p. 229) make the strong recommendation to transform to a scale where additivity more nearly obtains for purposes of estimation. This also reflects the motivation behind the famous Box and Cox (1964) family of transformations.

Of course, greater emphasis on linear models with Normal errors for observed potential outcomes can generate doubts as to whether randomization is necessary in experimental design. What is then lost is the fact that explicit randomization, as extolled by Fisher, provides the scientist with internally consistent statistical inferences that require no standard modeling assumptions, such as those required for linear regression. It is ironic that many textbooks on experimental design focus solely on Normal theory linear models, without realizing that such models were originally motivated as approximations for randomization inference.

Additivity has even been considered an essential assumption for interpreting estimands. For example, Cox (1958b, p. 16-17) states that the average difference in observed outcomes for two treatments estimates the difference in average potential outcomes for the two treatments in the finite population, but that this estimand of interest is *"... rather an artificial quantity"* if additivity does not hold on the potential outcomes. Perhaps Kempthorne (1952, p. 136) can best justify this statement

with the specific example where, for each experimental unit, the square root of the potential outcome under treatment is 5 more than the square root of the potential outcome under control. If one experimenter has three experimental units with control potential outcomes equal to $25, 64$ and 100, then the effect of the treatment on the raw measurement scale would range from 75 to 125. However, another experimenter working with units having control potential outcomes ranging from 9 to 16 would have treatment effects ranging from 55 to 65 on the raw scale. As Kempthorne states:

> Under these circumstances both experimenters will agree only if they state their results in terms of effects on the square root of the observation. It is desirable then to express effects on a scale of measurement such that they are exactly additive. (Kempthorne, 1952, p. 136)

Thus, Kempthorne's justification for additivity is that it enables externally consistent conclusions to be drawn from a particular analysis, i.e., two experimenters working with different samples from the same population will reach the same conclusion on the treatment effect. One could also interpret this as suggesting that experimenters should model the potential outcomes, with additive treatment effects being one simple model for an analysis.

Kempthorne continues to state that:

> Such a procedure has its defects, for experimenters prefer to state effects on a scale of measurement that is used as a matter of custom or for convenience reasons. It is probably difficult, for instance, to communicate to a farmer the meaning of the statement that a certain dose of an insecticide reduces the square root of the number of corn borers. A statement on the effect of number of corn borers can be made but is more complex. These difficulties are not, however, in the realm of the experimenter. He should examine his data on a scale of measurement which is such that treatment effects are additive. The real difficulty, in general, is to determine the scale of measurement that has the desired property. (Kempthorne, 1952, p. 136)

We again read in this quote the perceived importance of additivity that helped motivate the Box and Cox (1964) family of transformations. We do not believe it is necessary to study treatment effects on an additive scale: it is arguably more important to have an internally consistent definition and statistical procedure for studying treatment effects before deciding on externally consistent considerations. In our opinion, an ultimate consequence of this controversy is that, by focusing almost solely on linear models, advances in experimental design have been seriously inhibited from their original, useful, and liberating formulation involving potential outcomes.

1.4.2 Conclusions

The Neyman-Fisher controversy arose in part because Neyman sought to determine whether Fisher's ANOVA F-test for RCBs and LSs would still be valid when testing Neyman's more general null hypothesis. Unfortunately, Neyman's calculations were incorrect. In fact, under Neyman's conception of unbiased tests, the F-test for RCB designs potentially rejects at most at the nominal level, yet we could never know for any particular situation whether the F-test for LS designs would reject more often than nominal or not. Furthermore, Neyman's definition of unbiased tests is too crude, because expected mean sums of squares do not determine the Type I error of the F-test when testing Neyman's null. Two of the greatest statisticians argued over incorrect calculations and inexact measures of unbiasedness for hypothesis tests, adding an ironic aspect to this controversy.

What is also ironic is that apparently no statistician deigned to check Neyman's algebra or reasoning; the only discussant who suggested there was a mistake in Ney-

man's algebra was Fisher, but he did not explicitly state that Neyman was missing interactions in both expected mean residual sums of squares. Sukhatme (1935, p. 166, 167) recalculated the expected mean sums of squares in the general case where $\sigma^2_\eta(t)$ and $r(t,t')$ are not constant, and did not catch Neyman's mistake. Sukhatme also performed sampling experiments for two examples of LSs to support Neyman's claims. In both of Sukhatme's examples, there is no interaction between row/column blocking factors and treatment, so that $\mathbb{E}(S_0^2) < \mathbb{E}(S_1^2)$. Neyman (1935, p. 175) then considered his algebra correct, because *" ... none of my critics have attempted to challenge it."*

Fisher never referenced Neyman (1935) in his book on experimental design, and apparently ignored potential outcomes for many years (Rubin, 2005; Lehmann, 2011, p. 59). Fisher's avoidance of potential outcomes led him to make certain oversights in causal inference. In particular, as described by Rubin (2005), Fisher never bridged his work on experimental design and parametric modeling, and gave generally flawed advice on the analysis of covariance to adjust for posttreatment concomitants in randomized trials.

There is only one reference to Neyman (1935) by Hinkelmann and Kempthorne (2008, p. 387), and it was referred to as *"... an interesting somewhat different discussion ..."*. The standard accounts of Fisher and Neyman's professional careers (Box, 1978; Reid, 1982) do not mention any further work being done on questions raised by Neyman (1935), although Kempthorne is quoted as saying:

> The allusion to agriculture is quite unnecessary and the discussion is relevant to experimentation in any field of human enquiry. The discussion section ... is interesting because of the remarks of R.A. Fisher which are informative in some respects but in other respects exhibit Fisher at

> his very worst ... The judgement of the future will be, I believe, that Neyman's views were in the correct direction. (Reid, 1982, p. 123)

Even the recent account by Lehmann (2011, Chap. 4, 5) does not mention any statistician addressing Neyman's claims or checking his algebra. In fact, Lehmann ends his discussion of this controversy by recounting the destruction of the physical models Neyman used to illustrate his thoughts on RCB and LS designs during his 1935 presentation, thought to have been perpetrated by Fisher in a fit of anger (Reid, 1982, p. 124; Lehmann, 2011, Chap. 4).

We agree with Kempthorne's assessment that Neyman's views were in the correct direction in the following sense: by evaluating the frequency properties of statistics for both designs, one can see that the F-test is no longer precise without further assumptions on the potential outcomes. Such evaluations serve the important task of investigating the general properties of a design in a particular applied setting. The F-distribution is a useful approximation to the randomization distribution of the F-test statistic under Fisher's sharp null hypothesis and regularity conditions on the distribution of the potential outcomes or, alternatively for testing Neyman's null under additivity (Welch, 1937; Pitman, 1938).

We also agree with Cox (1958a) that, if block-treatment interactions are not negligible, then it is not particularly useful to test Neyman's null. More generally, we believe that one must think carefully about the type of null hypotheses one will test, and should be guided by an appropriate model on the potential outcomes. At one extreme, Fisher's sharp null hypothesis requires no model on the potential outcomes to test a reasonable, scientifically interesting null, with the reference distribution based solely on the randomization actually implemented during the experiment. To test

Neyman's null, one either needs strong regularity conditions on the potential outcomes for standard procedures to work, or one needs to think carefully to build and evaluate a model for the potential outcomes. In any case, one necessarily needs to make assumptions to assess more complicated null hypotheses, and it is important that assumptions on the potential outcomes are driven by actual science, routinely checked for their approximate validity, and not chosen based on necessary requirements for classical statistical procedures that have no real scientific merit.

Therefore, a better strategy than focusing on satisfying additivity to use the F-test for testing Neyman's null, we believe, is to introduce a Bayesian framework into the problem (Rubin, 1978). One can obtain a posterior predictive distribution for the estimand of interest (defined in terms of the potential outcomes) and evaluate relevant Bayes' rules using the same criteria that Neyman and others have considered (e.g., consistency, coverage, Type I error) (Rubin, 1984). The Fisher randomization test can be viewed as a type of posterior predictive check (Rubin, 1984), and it can be more enlightening (as the example in Section 1.3.2 illustrates) to perform explicitly the Fisher randomization test for Fisher's sharp null, rather than using the F-distribution as an approximation when testing Neyman's null under additivity. When additivity may not hold, evaluating Bayes' rules motivated by the particular applied setting of a problem appears to be a more viable path to the solution of a specific problem than relying on classical statistical procedures that are imprecise without applied contexts.

Chapter 2

Indicator Functions and the Algebra of the Linear-Quadratic Parameterization

2.1 Introduction

2.1.1 The Utility of the Linear-Quadratic Parameterization

Fractional factorial designs help address the challenge of screening and estimating main effects and interactions simultaneously for experiments with many factors and run size constraints. An important issue in their construction and subsequent analysis is the parameterization for factorial effects. The orthogonal components system (Wu and Hamada, 2009, p. 274) is a standard parameterization that facilitates calculations of design properties for regular fractions. However, it has two major disadvantages:

it can induce a simple aliasing structure, with any two contrasts either perfectly correlated or orthogonal (Ye, 2004), and it does not yield substantive interpretations for interaction components of quantitative factors.

These facts are illustrated in the example of a 3^{4-1}_{IV} design with quantitative factors (Wu and Hamada, 2009, p. 267–269, 281). If a pair of aliased two-factor interactions is judged significant in its orthogonal components analysis, then conclusive inferences on specific interactions cannot be made without further runs. One alternative system that does yield conclusive inferences and interpretable contrasts is the linear-quadratic system, generated by reparametrizing the factor levels using orthogonal polynominals (Wu and Hamada, 2009, p. 61, 287–288). The capacity for estimating two-factor interactions is better under the linear-quadratic system (Wu and Hamada, 2009, p. 292–293) because they are only partially aliased, in the sense that the absolute correlation of any pair of two-factor interaction contrasts is strictly less than 1. Although this design is regular, i.e., constructed by aliasing relations in a finite field, the linear-quadratic system yields a nonregular analysis through the introduction of partial aliasing. This enables a sequential strategy for de-aliasing factorial effects and identifying significant interactions that would otherwise be missed, with no need for further runs (Hamada and Wu, 1992; Wu and Hamada, 2009, p. 292). For all these reasons, the linear-quadratic system is preferable to orthogonal components.

However, the mathematics of the linear-quadratic system are not yet as transparent as the field theory basis for orthogonal components. A better understanding of the partial aliasing properties of this system is achieved with the indicator function of a design, and the focus of the current paper is to further develop the theory of

indicator functions under the linear-quadratic system.

2.1.2 Previous Applications of Indicator Functions

Based on the algebraic perspective of Pistone and Wynn (1996), Fontana et al. (2000) introduced the indicator function of unreplicated two-level fractional factorials, and proved the important fact that indicator function coefficients describe correlations between contrasts. Both Ye (2004) and Pistone and Rogantin (2008) considered indicator functions for designs with factors having more than two levels, and coded the levels by the complex roots of unity. A complex coding may be concise and amenable for generalizations to different settings, but we instead code factor levels with orthogonal polynomials, which may ultimately be used when fitting a model for the response, e.g., as in response surface methodology. Cheng and Ye (2004) considered indicator functions under the linear-quadratic system, and defined the concept of geometric isomorphism to consider changes in design properties corresponding to permutations in factor levels.

2.2 Indicator Functions under the Linear-Quadratic Parameterization

Let $\mathcal{D}$ be a 3^s full factorial, with the levels of factors $A_1, \ldots, A_s$ denoted by $-1, 0, 1$, corresponding to $0, 1, 2$ modulo 3 in the standard field notation. Field theory succinctly describes certain designs, and so it is necessary to move between these two notations. For example, when translating the regular fraction in Table 2.1 into linear-

quadratic notation, runs having A_1 at level 0 and A_2 at level 1 must have A_3 at level -1 in the linear-quadratic system, corresponding to $1 + 2 = 0$ modulo 3 in the field notation. It is also necessary to refer to orthogonal arrays having N runs, s factors, each with three levels, and strength t, and they are abbreviated as $\text{OA}(N, s, 3, t)$.

Table 2.1: Design with $A_3 = A_1 + A_2$ modulo 3. Three columns on the left represent the design under field notation, and the three on the right represent it using linear-quadratic notation.

Field Theory			Linear-Quadratic		
A_1	A_2	A_3	A_1	A_2	A_3
0	0	0	-1	-1	-1
0	1	1	-1	0	0
0	2	2	-1	1	1
1	0	1	0	-1	0
1	1	2	0	0	1
1	2	0	0	1	-1
2	0	2	1	-1	1
2	1	0	1	0	-1
2	2	1	1	1	0

The indicator function $F : \{-1, 0, 1\}^s \to \{0, 1\}$ for a fraction $\mathcal{F} \subseteq \mathcal{D}$ is the mapping with $F(x) = 1$ if $x \in \mathcal{F}$ and 0 otherwise, which can be extended for replicated runs using the generalized indicator function (Ye, 2003). This function is expressed as a unique linear combination of orthogonal contrast functions under the linear-quadratic system (Cheng and Ye, 2004). For each $i \in \{1, \ldots, s\}$, functions $X_{i,\text{L}}$, $X_{i,\text{Q}} : \mathbb{R}^s \to \mathbb{R}$ are defined as

$$X_{i,\text{L}}(x) = x_i, \quad X_{i,\text{Q}}(x) = 3x_i^2 - 2.$$

These correspond to linear and quadratic contrasts for the main effect of A_i (Wu and Hamada, 2009, p. 287). For distinct $i_1, \ldots, i_k \in \{1, \ldots, s\}$, and any $T_1, \ldots, T_k \in$

$\{\mathrm{L}, \mathrm{Q}\}$, define

$$X_{i_1 \cdots i_k, T_1 \cdots T_k}(x) = \prod_{j=1}^{k} X_{i_j, T_j}(x), \tag{2.2.1}$$

which corresponds to the $T_1 \cdots T_k$ interaction contrast of $A_{i_1}, \ldots, A_{i_k}$. Define $X_{\phi,\phi}(x) \equiv 1$, corresponding to the overall average. Functions $\{X_{I,T}(x) : I \in \mathcal{P},\ T \in \mathcal{T}_I\}$ form an orthogonal basis for $\mathcal{D}$, where $\mathcal{P}$ is the set of all concatenations of distinct elements from $\{1, \ldots, s\}$, and $\mathcal{T}_I$ is the set of all concatenations of $|I|$ elements from $\{\mathrm{L}, \mathrm{Q}\}$. This is summarized by the following lemma, given by Fontana et al. (2000) for two-level designs, and Cheng and Ye (2004).

Lemma 2.2.1. *For $I_1, I_2 \in \mathcal{P}$ and $T_1 \in \mathcal{T}_{I_1},\ T_2 \in \mathcal{T}_{I_2}$, $\sum_{x \in \mathcal{D}} X_{I_1,T_1}(x) X_{I_2,T_2}(x) \neq 0$ if and only if $I_1 = I_2,\ T_1 = T_2$.*

Lemma 2.2.1 implies that the indicator function is a unique linear combination of basis functions in (2.2.1): there exist unique $b_{I,T} \in \mathbb{R}$ for all $I \in \mathcal{P}, T \in \mathcal{T}_I$ such that

$$F(x) = \sum_{I \in \mathcal{P}} \sum_{T \in \mathcal{T}_I} b_{I,T} X_{I,T}(x). \tag{2.2.2}$$

Partial aliasing relations can be read from the indicator function coefficients $b_{I,T}$. The correlation of two contrasts having distinct factors is positively proportional to the coefficient involving all the factors, and correlations between contrasts involving the same factors are simple functions of these coefficients.

Calculation of the $b_{I,T}$ will be demonstrated later. At this point, the indicator function for the design in Table 2.1 is given to illustrate how representation (2.2.2) is

connected to partial aliasing:

$$\begin{aligned} F(x) = \frac{1}{3} &- \frac{3}{8}x_1x_2x_3 - \frac{1}{8}x_1x_2(3x_3^2-2) + \frac{1}{8}x_1(3x_2^2-2)x_3 - \frac{1}{8}x_1(3x_2^2-2)(3x_3^2-2) \\ &+ \frac{1}{8}(3x_1^2-2)x_2x_3 - \frac{1}{8}(3x_1^2-2)x_2(3x_3^2-2) + \frac{1}{8}(3x_1^2-2)(3x_2^2-2)x_3 \\ &+ \frac{1}{24}(3x_1^2-2)(3x_2^2-2)(3x_3^2-2). \end{aligned}$$

Coefficients involving one or two factors are zero precisely because the contrasts involved are orthogonal in this design. For example, $b_{12,\mathrm{LL}} = 0$ because the linear main effect of A_1, denoted by $(A_1)_\mathrm{L}$, is orthogonal to the linear main effect of A_2, $(A_2)_\mathrm{L}$. Alternatively, these coefficients are zero because the contrasts represented by these basis functions are valid, in the sense that they are orthogonal to the vector of ones. Thus, $b_{12,\mathrm{LL}} = 0$ because the two-factor linear-linear interaction between A_1 and A_2, i.e., the difference in the conditional linear effects of A_2 between the high and low levels of A_1 (Wu and Hamada, 2009, p. 288), denoted by $(A_1A_2)_\mathrm{LL}$, is orthogonal to $(1,\ldots,1)' \in \mathbb{R}^9$. Also, the correlation between $(A_1A_2)_\mathrm{LL}$ and $(A_3)_\mathrm{L}$ is proportional to $b_{123,\mathrm{LLL}} = -3/8$, and the correlation between $(A_1A_2)_\mathrm{LL}$ and $(A_1A_3)_\mathrm{LL}$ is proportional to $b_{123,\mathrm{QLL}} + b_{23,\mathrm{LL}} = 1/8$, with different, but positive, proportionality constants for both.

2.3 The Kronecker Product Operation on Factors

Calculation of indicator function coefficients involving all linear effects is accomplished by Corollary 2.2 in Cheng and Ye (2004). The following proposition summarizes a new calculation for coefficients involving at least one quadratic effect. All

proofs are in the appendix.

Proposition 2.3.1. *For distinct* $i_1, \ldots, i_k \in \{1, \ldots, s\}$, *and* $T_1, \ldots, T_k \in \{\mathrm{L}, \mathrm{Q}\}$ *with* $T_1, \ldots, T_j = \mathrm{L}$, $T_{j+1}, \ldots, T_k = \mathrm{Q}$, *and* $j = 1, \ldots, k-1$, *define*

$$B_{i_1 \cdots i_k, T_1 \cdots T_k} = \begin{cases} b_{i_1 \cdots i_j, T_1 \cdots T_j}, \ k = j+1, \\ b_{i_1 \cdots i_j, T_1 \cdots T_j} \\ \quad + \sum_{m=1}^{k-j-1} \left(\sum_{\substack{l_1, \ldots, l_m \in \{j+1, \ldots, k\}: \\ l_1 < \cdots < l_m}} b_{i_1 \cdots i_j i_{l_1} \cdots i_{l_m}, T_1 \cdots T_j T_{l_1} \cdots T_{l_m}} \right), \ k > j+1. \end{cases}$$

Then

$$b_{i_1 \cdots i_k, T_1 \cdots T_k} = 2^{-k} 3^{k-s} \sum_{x \in \mathcal{F}} X_{i_1, \mathrm{L}}(x)^{a_1} \cdots X_{i_k, \mathrm{L}}(x)^{a_k} - B_{i_1 \cdots i_k, T_1 \cdots T_k}, \tag{2.3.1}$$

where $a_1 = \cdots = a_j = 1$, *and* $a_{j+1} = \cdots = a_k = 2$.

Also, define

$$B_{i_1 \cdots i_k, \mathrm{Q} \cdots \mathrm{Q}} = b_{\phi, \phi} + \sum_{m=1}^{k-1} \left(\sum_{\substack{l_1, \ldots, l_m \in \{1, \ldots, k\}: \\ l_1 < \cdots < l_m}} b_{i_{l_1} \cdots i_{l_m}, \mathrm{Q} \cdots \mathrm{Q}} \right).$$

Then

$$b_{i_1 \cdots i_k, \mathrm{Q} \cdots \mathrm{Q}} = 2^{-k} 3^{k-s} \sum_{x \in \mathcal{F}} X_{i_1, \mathrm{L}}(x)^2 \cdots X_{i_k, \mathrm{L}}(x)^2 - B_{i_1 \cdots i_k, \mathrm{Q} \cdots \mathrm{Q}}. \tag{2.3.2}$$

There are three points to note. First, Proposition 2.3.1 involves $b_{\phi, \phi} = |\mathcal{F}|/3^s$ (Cheng and Ye, 2004). Second, it connects low-order and high-order coefficients,

and shows how factors with linear effects carry through. If a set of factors form an orthogonal array of strength t, then all coefficients involving t or fewer of these factors are zero. As described later, the combination of this fact with Proposition 2.3.1 illuminates calculations of a design's properties. Third, if interest lies in specific high-order coefficients, the calculation method of Cheng and Ye (2004, p. 2173) is better.

To demonstrate Proposition 2.3.1, consider Table 2.1. This is an orthogonal array of strength 2, so $b_{i_1,T_1} = b_{i_1 i_2,T_1 T_2} = 0$ for distinct $i_1, i_2 \in \{1,2,3\}$, and any $T_1,\ T_2 \in \{\mathrm{L},\mathrm{Q}\}$. Then

$$\begin{aligned}
b_{123,\mathrm{LLQ}} &= \frac{1}{8}\sum_{x\in\mathcal{F}} X_{1,\mathrm{L}}(x)X_{2,\mathrm{L}}(x)X_{3,\mathrm{L}}(x)^2 = -\frac{1}{8},\\
b_{123,\mathrm{LQQ}} &= \frac{1}{8}\sum_{x\in\mathcal{F}} X_{1,\mathrm{L}}(x)X_{2,\mathrm{L}}(x)^2X_{3,\mathrm{L}}(x)^2 = -\frac{1}{8},\\
b_{123,\mathrm{QQQ}} &= \frac{1}{8}\sum_{x\in\mathcal{F}} X_{1,\mathrm{L}}(x)^2X_{2,\mathrm{L}}(x)^2X_{3,\mathrm{L}}(x)^2 - b_{\phi,\phi} = \frac{3}{8} - \frac{1}{3} = \frac{1}{24}.
\end{aligned}$$

This shows how Proposition 2.3.1 eliminates the need to deal with quadratic contrast functions.

Proposition 2.3.1 is used to define an operation for factors under the linear-quadratic system that enables one to read from the design in linear-quadratic notation to calculate the $b_{I,T}$. For any $i \in \{1,\ldots,s\}$, define $\mathcal{F}_{i,\mathrm{L}} = \{x \in \mathcal{F} : x_i = 1\}$, $\mathcal{F}_{i,\mathrm{Q}} = \{x \in \mathcal{F} : x_i = -1\}$. By Proposition 2.3.1,

$$\begin{pmatrix} b_{i,\mathrm{L}} \\ b_{i,\mathrm{Q}} \end{pmatrix} = 2^{-1}3^{1-s}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} |\mathcal{F}_{i,\mathrm{L}}| \\ |\mathcal{F}_{i,\mathrm{Q}}| \end{pmatrix} - \begin{pmatrix} 0 \\ b_{\phi,\phi} \end{pmatrix}.$$

Coefficients for factors A_{i_1} and A_{i_2} are then obtained by a scaled Kronecker product of Hadamard matrices, and an intersection of the sets defined above, again by Proposition 2.3.1. Specifically, defining $\mathcal{F}_{i_1 i_2, T_1 T_2} = \mathcal{F}_{i_1, T_1} \bigcap \mathcal{F}_{i_2, T_2}$ for any $T_1, T_2 \in \{\mathrm{L}, \mathrm{Q}\}$,

$$\begin{pmatrix} b_{i_1 i_2,\mathrm{LL}} \\ b_{i_1 i_2,\mathrm{LQ}} \\ b_{i_1 i_2,\mathrm{QL}} \\ b_{i_1 i_2,\mathrm{QQ}} \end{pmatrix} = 2^{-2} 3^{2-s} \left\{ \bigotimes_{j=1}^{2} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \right\} \begin{pmatrix} |\mathcal{F}_{i_1 i_2,\mathrm{LL}}| \\ |\mathcal{F}_{i_1 i_2,\mathrm{LQ}}| \\ |\mathcal{F}_{i_1 i_2,\mathrm{QL}}| \\ |\mathcal{F}_{i_1 i_2,\mathrm{QQ}}| \end{pmatrix} - \begin{pmatrix} 0 \\ B_{i_1 i_2,\mathrm{LQ}} \\ B_{i_1 i_2,\mathrm{QL}} \\ B_{i_1 i_2,\mathrm{QQ}} \end{pmatrix}.$$

We formally define $A_{i_1} \otimes A_{i_2} = (b_{i_1 i_2,\mathrm{LL}}, b_{i_1 i_2,\mathrm{LQ}}, b_{i_1 i_2,\mathrm{QL}}, b_{i_1 i_2,\mathrm{QQ}})'$.

This operation is easily extended to more than two factors: $A_{i_1} \otimes \cdots \otimes A_{i_k}$ is defined as the vector of indicator function coefficients, in a lexicographic ordering of linear and quadratic effects, involving all these k distinct factors. To write this explicitly, define $\mathcal{F}_{i_1 \cdots i_k, T_1 \cdots T_k} = \bigcap_{j=1}^{k} \mathcal{F}_{i_j, T_j}$ for any $T_{i_1}, \ldots, T_{i_k} \in \{\mathrm{L}, \mathrm{Q}\}$. Then, by Proposition 1,

$$A_{i_1} \otimes \cdots \otimes A_{i_k} = 2^{-k} 3^{k-s} \left\{ \bigotimes_{j=1}^{k} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \right\} \begin{pmatrix} |\mathcal{F}_{i_1 \cdots i_{(k-1)} i_k,\mathrm{L}\cdots\mathrm{LL}}| \\ |\mathcal{F}_{i_1 \cdots i_{(k-1)} i_k,\mathrm{L}\cdots\mathrm{LQ}}| \\ |\mathcal{F}_{i_1 \cdots i_{(k-1)} i_k,\mathrm{L}\cdots\mathrm{QL}}| \\ |\mathcal{F}_{i_1 \cdots i_{(k-1)} i_k,\mathrm{L}\cdots\mathrm{QQ}}| \\ \vdots \\ |\mathcal{F}_{i_1 \cdots i_{(k-1)} i_k,\mathrm{Q}\cdots\mathrm{LL}}| \\ |\mathcal{F}_{i_1 \cdots i_{(k-1)} i_k,\mathrm{Q}\cdots\mathrm{LQ}}| \\ |\mathcal{F}_{i_1 \cdots i_{(k-1)} i_k,\mathrm{Q}\cdots\mathrm{QL}}| \\ |\mathcal{F}_{i_1 \cdots i_{(k-1)} i_k,\mathrm{Q}\cdots\mathrm{QQ}}| \end{pmatrix} - \begin{pmatrix} 0 \\ B_{i_1 \cdots i_{(k-1)} i_k,\mathrm{L}\cdots\mathrm{LQ}} \\ B_{i_1 \cdots i_{(k-1)} i_k,\mathrm{L}\cdots\mathrm{QL}} \\ B_{i_1 \cdots i_{(k-1)} i_k,\mathrm{L}\cdots\mathrm{QQ}} \\ \vdots \\ B_{i_1 \cdots i_{(k-1)} i_k,\mathrm{Q}\cdots\mathrm{LL}} \\ B_{i_1 \cdots i_{(k-1)} i_k,\mathrm{Q}\cdots\mathrm{LQ}} \\ B_{i_1 \cdots i_{(k-1)} i_k,\mathrm{Q}\cdots\mathrm{QL}} \\ B_{i_1 \cdots i_{(k-1)} i_k,\mathrm{Q}\cdots\mathrm{QQ}} \end{pmatrix}.$$

Thus, counts of ± 1 level combinations are sufficient for calculating indicator function coefficients under the linear-quadratic system. Applying an affine transformation to these counts by first performing a scaled rotation, corresponding to the scaled Hadamard matrix built by the Kronecker product, and then a shift by coefficients of lower order, consisting of factors with linear effects and subsets of factors with quadratic effects, yields coefficients involving all factors of interest. This suggests a geometric view, with affine transformations of counts of runs determining partial aliasing properties. Fontana (2013) provides another view on Kronecker products.

Example 2.3.2. Consider the design in Table 2.2. As this is an orthogonal array of strength 2, nonzero indicator coefficients must involve at least three factors. By counting the $|\mathcal{F}_{123,T_1T_2T_3}|$,

$$\begin{aligned} A_1 \otimes A_2 \otimes A_3 &= 2^{-3}3^{-1} \left\{ \bigotimes_{j=1}^{3} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \right\} (0,0,1,0,1,0,0,1)' - \left(0,0,0,0,0,0,0,\frac{1}{9}\right)' \\ &= \left(-\frac{1}{8}, -\frac{1}{24}, \frac{1}{24}, -\frac{1}{24}, \frac{1}{24}, -\frac{1}{24}, \frac{1}{24}, \frac{1}{72}\right)'. \end{aligned}$$

Similar computations are performed for $A_1 \otimes A_2 \otimes A_4$, $A_1 \otimes A_3 \otimes A_4$ and $A_2 \otimes A_3 \otimes A_4$, leading to the result that $A_1 \otimes A_2 \otimes A_3 \otimes A_4 = (0, \ldots, 0)'$. Thus, two-factor interactions involving distinct factors are orthogonal in this design.

Example 2.3.3. Construction of an $\text{OA}(18, 6, 3, 2)$ by the Kronecker sum operation on a difference matrix (Wang and Wu, 1991) makes calculation of the indicator function

Table 2.2: Design with $A_3 = A_1 + A_2$, $A_4 = A_1 + 2A_2$ modulo 3. Four columns on the left represent it under field notation, and the four on the right represent it using linear-quadratic notation.

Field Theory				Linear-Quadratic			
A_1	A_2	A_3	A_4	A_1	A_2	A_3	A_4
0	0	0	0	-1	-1	-1	-1
0	1	1	2	-1	0	0	1
0	2	2	1	-1	1	1	0
1	0	1	1	0	-1	0	0
1	1	2	0	0	0	1	-1
1	2	0	2	0	1	-1	1
2	0	2	2	1	-1	1	1
2	1	0	1	1	0	-1	0
2	2	1	0	1	1	0	-1

particularly enlightening. The difference matrix $D_{6,6;3}$ is defined as

$$D_{6,6;3} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 2 & 0 & 1 & 2 \\ 0 & 2 & 1 & 1 & 0 & 2 \\ 0 & 0 & 2 & 1 & 2 & 1 \\ 0 & 2 & 0 & 2 & 1 & 1 \\ 0 & 1 & 1 & 2 & 2 & 0 \end{pmatrix},$$

and the array is constructed by the following transformation involving addition modulo 3:

$$\begin{pmatrix} D_{6,6;3} \\ D_{6,6;3} + J \text{ modulo } 3 \\ D_{6,6;3} + 2J \text{ modulo } 3 \end{pmatrix},$$

where J is the 6×6 matrix with all entries equal to 1. The correspondence between runs 7–12 and 1–6, and also between runs 13–18 and 1–6, illuminates the calculation

of indicator function coefficients. For example, for distinct factors i_1, i_2, i_3,

$$|\mathcal{F}_{i_1 i_2 i_3,\mathrm{LLL}}| = |\mathcal{F}_{i_1 i_2 i_3,\mathrm{QQQ}}| = \sum_{\substack{x \in D_{6,6;3}: \\ x_{i_1} = x_{i_2} = x_{i_3}}} 1 = 1.$$

In addition,

$$|\mathcal{F}_{i_1 i_2 i_3,\mathrm{LLQ}}| = \sum_{\substack{x \in D_{6,6;3}: \\ x_{i_1} = x_{i_2}, \\ x_{i_3} = x_{i_1} + 1}} 1, \quad |\mathcal{F}_{i_1 i_2 i_3,\mathrm{QQL}}| = \sum_{\substack{x \in D_{6,6;3}: \\ x_{i_1} = x_{i_2}, \\ x_{i_3} = x_{i_1} + 2}} 1.$$

From the definition of a difference matrix,

$$\sum_{\substack{x \in D_{6,6;3}: \\ x_{i_1} = x_{i_2}}} 1 \quad = \quad \sum_{\substack{x \in D_{6,6;3}: \\ x_{i_1} = x_{i_2} = x_{i_3}}} 1 \quad + \quad \sum_{\substack{x \in D_{6,6;3}: \\ x_{i_1} = x_{i_2}, \\ x_{i_3} = x_{i_1} + 1}} 1 \quad + \quad \sum_{\substack{x \in D_{6,6;3}: \\ x_{i_1} = x_{i_2}, \\ x_{i_3} = x_{i_1} + 2}} 1 \quad = \quad 2,$$

hence $|\mathcal{F}_{i_1 i_2 i_3,\mathrm{QQL}}| = 1 - |\mathcal{F}_{i_1 i_2 i_3,\mathrm{LLQ}}|$. Similarly, $|\mathcal{F}_{i_1 i_2 i_3,\mathrm{QLQ}}| = 1 - |\mathcal{F}_{i_1 i_2 i_3,\mathrm{LQL}}|$ and $|\mathcal{F}_{i_1 i_2 i_3,\mathrm{QLL}}| = 1 - |\mathcal{F}_{i_1 i_2 i_3,\mathrm{LQQ}}|$. Thus, only $|\mathcal{F}_{i_1 i_2 i_3,\mathrm{LLL}}|, |\mathcal{F}_{i_1 i_2 i_3,\mathrm{LLQ}}|, |\mathcal{F}_{i_1 i_2 i_3,\mathrm{LQL}}|$, and $|\mathcal{F}_{i_1 i_2 i_3,\mathrm{LQQ}}|$ are necessary to calculate $A_{i_1} \otimes A_{i_2} \otimes A_{i_3}$, and each is 0 or 1, as determined by $D_{6,6;3}$ in the manner described above.

These calculations highlight an analogy between the construction of a design and its analysis under the linear-quadratic system, and the construction of regular fractional factorials and their analysis under orthogonal components. Field theory provides both a method to construct designs, namely, regular fractions, and a corresponding method of analysis, the orthogonal components system, that facilitates calculations of aliasing relations. For the linear-quadratic system, calculations for indicator coefficients, hence partial aliasing relations, are built through the $\otimes$ operation in a similar manner for designs constructed by transformations of generators,

e.g., orthogonal arrays based on difference matrices. Constructing a design through its rows is important for the linear-quadratic system, and such designs, referred to as row generator-transformation designs, are to the linear-quadratic system as regular fractions are to orthogonal components. Cheng and Wu (2001) and Bulutoglu and Cheng (2003) provide further examples of such designs.

2.4 Partial Aliasing Relations for OA$(3^n, s, 3, n)$

Proposition 2.3.1 aids in the exploration of partial aliasing relations in OA$(3^n, s, 3, n)$ by facilitating derivations of relationships among indicator function coefficients. It is used to prove that coefficients for any $n+1$ factors are invariant to permutation of linear and quadratic effects in absolute value, and that coefficients for any $n+2$ factors are zero.

Proposition 2.4.1. *For factors $A_1, \ldots, A_{n+1}$ in an* OA*$(3^n, s, 3, n)$ and $T_1, \ldots, T_{n+1} \in \{\mathrm{L}, \mathrm{Q}\}$,*

$$|b_{1\cdots(n+1),T_1\cdots T_{n+1}}| = |b_{1\cdots(n+1),T_{\psi(1)}\cdots T_{\psi(n+1)}}|$$

for any permutation ψ on $\{1, \ldots, n+1\}$.

Corollary 2.4.2. *For a design with $A_{n+1} = c_0 + c_1A_1 + \cdots + c_nA_n$* modulo 3*, where $A_1, \ldots, A_n$ form an orthogonal array of strength n and $c_0, \ldots, c_n \in \{0, 1, 2\}$,*

$$|b_{1\cdots(n+1),T_1\cdots T_{n+1}}| = |b_{1\cdots(n+1),T_{\psi(1)}\cdots T_{\psi(n+1)}}|$$

for any $T_1, \ldots, T_{n+1} \in \{\mathrm{L}, \mathrm{Q}\}$ and permutation ψ on $\{1, \ldots, n+1\}$.

To illustrate this for Table 1, $|b_{123,\mathrm{LLQ}}| = |b_{123,\mathrm{LQL}}| = |b_{123,\mathrm{QLL}}|$ and $|b_{123,\mathrm{LQQ}}| = |b_{123,\mathrm{QLQ}}| = |b_{123,\mathrm{QQL}}|$. If a design had $b_{123,\mathrm{LLQ}} = 0$, with A_1, A_2, and A_3 forming a defining relation, then all two-factor linear-linear interactions are uncorrelated with a quadratic main effect, or alternatively all two-factor linear-quadratic interactions are uncorrelated with a linear main effect, for these factors. For each set of $n+1$ factors in an $\mathrm{OA}(3^n, s, 3, n)$, their coefficients can be partitioned according to the number of linear and quadratic effects, and their estimable interactions correspond to a $b_{I,T}$ equal to zero and permutations of effects in T.

Proposition 2.4.3. *In an* $\mathrm{OA}(3^n, s, 3, n)$, $A_1 \otimes \cdots \otimes A_{n+2} = (0, \ldots, 0)'$.

Corollary 2.4.4. *For a design with*

$$A_{n+1} = c_0 + c_1 A_1 + \cdots + c_n A_n \text{ modulo } 3,$$

$$A_{n+2} = d_0 + d_1 A_1 + \cdots + d_n A_n \text{ modulo } 3,$$

where $A_1, \ldots, A_n$ *form an orthogonal array of strength* n, *and* $c_0, \ldots, c_n, d_0, \ldots, d_n \in \{0, 1, 2\}$ *with* $c_1, \ldots, c_n, d_1, \ldots, d_n \neq 0$,

$$A_1 \otimes \cdots \otimes A_{n+2} = (0, \ldots, 0)'.$$

These results show how two-factor interactions can be orthogonal to n-factor interactions. Another interpretation is of main effects being orthogonal to $(n+1)$-factor interactions, if they are valid contrasts. Proposition 2.4.3 further eliminates the need to calculate indicator function coefficients guaranteed to be zero for certain designs.

2.5 Conditions for Estimable Interactions

Conditions that yield estimable interactions are now considered. As before, Proposition 2.3.1 is instrumental in proving these results.

Proposition 2.5.1. *For factors A_1, A_2, A_3 forming an orthogonal array of strength 2 in $\mathcal{F}$, $b_{123,T_1T_2\mathrm{L}} = 0$ for all $T_1, T_2 \in \{\mathrm{L}, \mathrm{Q}\}$ if and only if $|\mathcal{F}_{123,T_1T_2\mathrm{L}}| = |\mathcal{F}_{123,T_1T_2\mathrm{Q}}|$ for all $T_1, T_2 \in \{\mathrm{L}, \mathrm{Q}\}$, and it is impossible for $b_{123,T_1T_2\mathrm{Q}} = 0$ for all $T_1, T_2 \in \{\mathrm{L}, \mathrm{Q}\}$ if $|\mathcal{F}|/9$ is not divisible by 3.*

Proposition 2.5.2. *For factors A_1, A_2, A_3 forming an orthogonal array of strength 2 in $\mathcal{F}$, if*

$$\sum_{\substack{x \in \mathcal{F}: \\ x_1x_2=1}} X_{3,\mathrm{L}}(x) = \sum_{\substack{x \in \mathcal{F}: \\ x_1x_2=-1}} X_{3,\mathrm{L}}(x) = 0,$$

then $b_{123,\mathrm{LLL}} = b_{123,\mathrm{QQL}} = 0$. Furthermore, if these factors form a defining relation, then $b_{123,\mathrm{QLQ}} = b_{123,\mathrm{LQQ}} = 0$.

Proposition 2.5.1 gives a necessary and sufficient condition for $(A_3)_\mathrm{L}$ to be orthogonal to all two-factor interactions $(A_1A_2)_{T_1T_2}$, and a necessary condition for $(A_3)_\mathrm{Q}$ to be orthogonal to all $(A_1A_2)_{T_1T_2}$. Proposition 2.5.2 differs from Proposition 2.5.1 because it considers a specific structure on the runs that yields uncorrelated main effects and two-factor interactions. It has the following practical implication: for quantitative factors, with -1 and 1 being the smallest and largest levels, respectively, for each, uncorrelated main effects and two-factor interactions are achievable by having symmetry in a subset of runs. This is expressed in field notation in the following corollary.

Corollary 2.5.3. *For factors* A_1, A_2, A_3 *with* $A_3 = d_1A_1 + d_2A_2$ modulo 3 *in* $\mathcal{F}$, $b_{123,\text{LLL}} = b_{123,\text{QQL}} = b_{123,\text{LQQ}} = b_{123,\text{QLQ}} = 0$ *if and only if* $d_1 = d_2 = 2$ modulo 3.

One may need to design an experiment in which the effect hierarchy principle (Wu and Hamada, 2009, p. 172) is violated, e.g., some factors are more important through two-factor interactions. The following proposition introduces a design construction technique for the linear-quadratic system that can be useful in such situations.

Proposition 2.5.4. *If* $A_{n+2} = c_0 + c_1A_1 + \cdots + c_nA_n$ modulo 3*, and* $A_1, \ldots, A_n, A_{n+1}$ *form an orthogonal array of strength* $n+1$*, then* $A_1 \otimes \cdots \otimes A_{n+1} \otimes A_{n+2} = (0, \ldots, 0)'$.

Corollary 2.5.5. *If*

$$A_j = c_0 + c_1A_1 + \cdots + c_nA_n \text{ modulo } 3,$$

$$A_{j\prime} = d_0 + d_1A_1 + \cdots + d_nA_n + d_{n+1}A_{n+1} + \cdots + d_{n+m}A_{n+m} \text{ modulo } 3,$$

where at least one of $d_{n+i} \neq 0$ *modulo* 3 *for* $i = 1, \ldots, m$*, and* $A_1, \ldots, A_{n+m}$ *form an orthogonal array of strength* $n+m$*, then* $A_1 \otimes \cdots \otimes A_n \otimes A_j \otimes A_{j\prime} = (0, \ldots, 0)'$.

To illustrate the statistical relevance of these results, consider designing a three-level fractional factorial with four factors and 27 runs, in which interest is on two-factor interactions. For the 3^{4-1}_{IV} design with $A_4 = A_1 + A_2 + A_3$ modulo 3, certain two-factor interactions are fully aliased with other two-factor interactions under orthogonal components, and are only partially aliased under the linear-quadratic system. Now consider the design with aliasing relation $A_4 = 2A_1 + 2A_2$ modulo 3, with A_1, A_2, A_3 forming an orthogonal array of strength 3. From Corollary 2.5.3 and

Proposition 2.5.4, all two-factor interactions involving distinct factors are orthogonal, $(A_4)_{\mathrm{L}}$ is uncorrelated with $(A_1A_2)_{\mathrm{LL}}, (A_1A_2)_{\mathrm{QQ}}$, and $(A_4)_{\mathrm{Q}}$ is uncorrelated with $(A_1A_2)_{\mathrm{LQ}}, (A_1A_2)_{\mathrm{QL}}$. If the main effects of A_4 are not significant, we can entertain two-factor interactions involving distinct factors, and those involving the same factor will only be partially aliased. Proposition 2.5.4 and Corollary 2.5.5 offer the interesting possibility of high-order factorial effects being legitimate contrasts, while low-order effects are not: for this design, four-factor interactions are valid contrasts, whereas three-factor interactions of A_1, A_2, A_4 are not.

2.6 Concluding Remarks

The operation and results in this paper help in understanding properties of the linear-quadratic system. For example, Cheng and Ye (2004) provide a definition for the generalized wordlength pattern of a design that involves indicator function coefficients. By virtue of Proposition 2.3.1, an expression for the generalized wordlength pattern that makes explicit the contribution of low-order coefficients can be derived. As pointed out by a referee, our operation can be applied to qualitative factors as well, and any permutation in the coding of qualitative variables might lead to designs with different geometric characteristics and models (Cheng and Ye, 2004).

These results can also aid in deriving bounds on the magnitude of indicator function coefficients, hence on correlations among contrasts, because the $\otimes$ operation only requires counts of ± 1 level combinations. Similarly, calculation of bounds for D- and G-efficiencies should be simpler with this operation, and hence one can better explore and understand the eligibility of designs for factor screening and response surface

exploration (Cheng and Wu, 2001).

Recall that the linear-quadratic system is generated by reparametrizing the levels of quantitative factors using orthogonal polynomials. Accordingly, the results in this paper can be extended to designs with more than three levels per factor by means of orthogonal polynomials.

Examples presented here used standard field constructions for regular designs. As seen in Example 2.3.3, partial aliasing calculations are also transparent for row generator-transformation designs. The role of a design's construction in its analysis under the linear-quadratic system is an important question that warrants further investigation.

Chapter 3

Inference for Deformation and Interference in 3D Printing

3.1 Interference in Compensation

Additive manufacturing, or 3D printing, refers to a class of technology for the direct fabrication of physical products from 3D Computer-Aided Design (CAD) models. In contrast to material removal processes in traditional machining, the printing process adds material layer by layer. This enables direct printing of geometrically complex products without affecting building efficiency. No extra effort is necessary for molding construction or fixture tooling design, making 3D printing a promising manufacturing technique (Hilton and Jacobs, 2000; Gibson et al., 2009; Melchels et al., 2010; Campbell et al., 2011). Despite these promising features, control of a product's printed dimensions (i.e., dimensional accuracy control) remains a major bottleneck. Material solidification during layer formation leads to product deforma-

tion, or shrinkage (Wang et al., 1996), which reduces the utility of printed products. Shrinkage control is crucial to overcome the accuracy barrier in 3D printing.

To control detailed features along the boundary of a printed product, Tong et al. (2003) and Tong et al. (2008) used polynomial regression models to first analyze shrinkage in different directions separately, and then compensate for product deformation by changing the original CAD accordingly. Unfortunately, their predictions are independent of the product's geometry, which is not consistent with the physical manufacturing process. Huang et al. (2013) built on this work, using polar coordinates to develop a physically consistent approach to model and compensate for shrinkage. Validation experiments suggest that this approach can achieve greater accuracy control.

To control detailed features along the boundary of a printed product, Tong et al. (2003) and Tong et al. (2008) used polynomial regression models to first analyze shrinkage in different directions separately, and then compensate for product deformation by changing the original CAD accordingly. Unfortunately, their predictions are independent of the product's geometry, which is not consistent with the physical manufacturing process. Huang et al. (2013) built on this work, establishing a generic, physically consistent approach to model and predict product deformations, and to derive compensation plans that achieve dimensional accuracy control. The essence of this new modeling approach is to transform in-plane geometric errors from the Cartesian coordinate system into a functional profile defined on the polar coordinate system. This representation decouples the geometric shape complexity from the deformation modeling, and a generic formulation of shape deformations can thus be

achieved. The approach was developed for a stereolithography process, and in experiments achieved an improvement of one order of magnitude in reduction of deformation for cylinder products.

However, an important issue not yet addressed in the previously cited work on deformation control for 3D printing is how the application of compensation to one section of a product will affect the deformation of neighboring sections. Compensation plans are always discretized according to the tolerance of the 3D printer, in the sense that sections of the CAD are altered by single amounts, e.g., as in Figure 3.1. Furthermore, when planning an experiment to assess the effect of compensations on product deformation, it is natural to discretize the quantitative "compensation" factor into a finite number of levels, which also leads to a product having a more complex boundary. Ultimately, such changes may introduce interference between different sections of the printed product, which is defined to occur when one section's deformation depends not only on its assigned compensation, but also on compensations applied to its neighbors (Rubin, 1980). For example, in Figure 3.1, the deformation for points near the boundary of two neighboring sections should depend on compensations applied to both sections. By the same logic, interference becomes a practical issue when printing products with complex geometry. Therefore, to improve dimensional accuracy control in 3D printing, it is important to formally investigate complications introduced by the interference that results from the inevitable discretization in compensation plans. We take the first step with an experiment involving a discretized compensation plan for a simple geometric shape.

We begin in Section 3.2 with a review of interference, models for product defor-

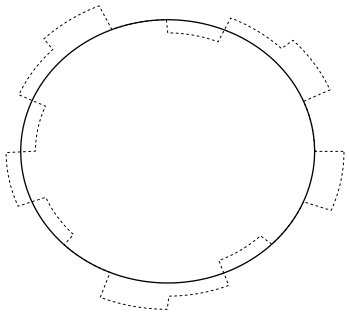

Figure 3.1: A discretized compensation plan (dashed-line) to the nominal boundary (solid line). Note that compensation could be negative.

mation, and the effect of compensation. Adoption of the Rubin Causal Model (RCM, Holland, 1986) is a significant and novel feature of our investigation in 3D printing, and it facilitates the study of interference. Section 3.3.1 summarizes the basic model and analysis for deformation of cylinders given by Huang et al. (2013). Our analyses are in Sections 3.3.2–3.3.5: we first describe an experimental design hypothesized to generate interference, then proceed with posterior predictive checks to demonstrate the existence of interference, and finally conclude with a model that captures interference. A statistically significant idea arising in Section 3.3.3 is that, in experiments explicitly making a distinction between *units of analysis* and *units of interpretation* (Cox and Donnelly, 2011, p. 18–19), the posterior distribution of model parameters, constructed using "benchmark" data, naturally leads to a simple assessment and inference for interference similar to that suggested by Sobel (2006) and Rosenbaum (2007). Analyses in Sections 3.3.4–3.3.5 demonstrate how discretized compensations complicate dimensional accuracy control along a product's boundary through the introduction of interference. This illustrates the fact that in complex manufacturing

processes, a proper definition of experimental units and understanding of how units may interfere with each other are critical to quality control.

3.2 Potential Outcomes and Interference

3.2.1 Definition of Experimental Units and Potential Outcomes

We use the general framework for product deformation given by Huang et al. (2013, p. 3–6). Suppose a product has intended shape ψ_0, and observed shape ψ under a 3D printing process. Deformation is informally described as the difference between ψ and ψ_0, where we can represent both either in the Cartesian coordinate system (x, y, z) or cylindrical coordinate system (r, θ, z). Cylindrical coordinates facilitate deformation modeling, and are used throughout.

For illustrative purposes, we define terms for two-dimensional products (notation for three dimensions follow immediately). Dimensional accuracy control requires an understanding of deformation in different regions of the product that receive different amounts of compensation. We therefore define a finite number N points on the boundary of the product, corresponding to specific angles $\theta_1, \ldots, \theta_N$, as the experimental units. The desired boundary from the CAD model is defined by the function $r_0(\theta)$, denoting the nominal radius at angle θ. We consider only one (quantitative) treatment factor, compensation to the CAD, defined as a change in the nominal radius of the CAD by x_i units at θ_i for $i = 1, \ldots, N$. The potential radius for θ_i under the application of treatments $\mathbf{x} = (x_1, \ldots, x_N)$ to units $\theta_1, \ldots, \theta_N$ is a function of

θ_i, $r_0(\cdot)$, and $\mathbf{x}$, denoted by $r(\theta_i, r_0(\cdot), \mathbf{x})$. The difference between the potential and nominal radius at θ_i defines deformation, and so we define

$$\Delta r(\theta_i, r_0(\cdot), \mathbf{x}) = r(\theta_i, r_0(\cdot), \mathbf{x}) - r_0(\theta_i) \tag{3.2.1}$$

as our *potential outcome* for θ_i. For now, potential outcomes are viewed as fixed numbers, with randomness introduced in Section 3.2.3 in our general model for the potential outcomes.

This definition of the potential outcome is convenient for visualizing shrinkage. For example, suppose the desired shape of the product is the solid line, and the manufactured product when $\mathbf{x} = \mathbf{0} = (0, \ldots, 0)$ is the dashed-line, in Figure 3.2. Plotting the deformation at each angle leads to a visualization amenable to analysis. Orientation is fixed: we match the coordinate axes of the printed product with those of the CAD model.

3.2.2 Interference

A unit θ_i is said to be affected by interference if

$$\Delta r(\theta_i, r_0(\cdot), \mathbf{x}) \neq \Delta r(\theta_i, r_0(\cdot), \mathbf{x}')$$

for at least one pair of distinct treatment vectors $\mathbf{x}, \mathbf{x}' \in \mathbb{R}^N$ with $x_i = x_i'$ (Rubin, 1980). If there is no interference, then

$$\Delta r(\theta_i, r_0(\cdot), \mathbf{x}) = \Delta r(\theta_i, r_0(\cdot), x_i).$$

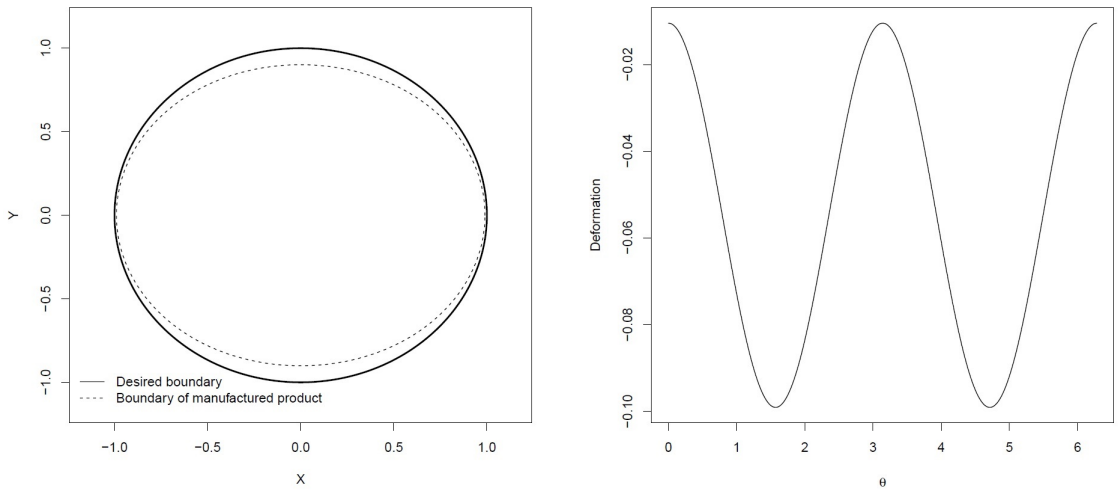

Figure 3.2: The left figure compares the ideal shape (solid line) with the actual shape (dashed-line). Shrinkage is visualized in the right figure.

As the experimental units reside on a connected boundary, the deformation of one unit may depend on compensations assigned to its neighbors when the compensation plan is discretized. Perhaps less plausible, but equally serious, is the leakage of assigned compensations across units. These considerations explain the presence of the vector $\mathbf{x}$, containing treatment assignments for all units, in the potential outcome notation (3.2.1). Practically, accommodations made for interference should reduce bias in compensation plans for complex products, and improve dimensional accuracy control.

3.2.3 General Deformation Model

Following Huang et al. (2013, p. 6–8), our potential outcome model under treatment assignment $\mathbf{x} = \mathbf{0}$ is decomposed into three components:

$$\Delta r(\theta_i, r_0(\cdot), \mathbf{0}) = f_1(r_0(\cdot)) + f_2(\theta_i, r_0(\cdot), \mathbf{0}) + \epsilon_i. \tag{3.2.2}$$

Function $f_1(r_0(\cdot))$ represents average deformation of a given nominal shape $r_0(\cdot)$ independent of location θ_i, and $f_2(\theta_i, r_0(\cdot), \mathbf{0})$ is the additional location-dependent deformation, geometrically and physically related to the CAD model. We can also interpret $f_1(\cdot)$ as a lower order component and $f_2(\cdot, \cdot, \mathbf{0})$ as a higher order component of deformation. The ϵ_i are random variables representing high frequency components that add on to the main trend, with expectation $\mathbb{E}(\epsilon_i) = 0$ and $\text{Var}(\epsilon_i) < \infty$ for all $i = 1, \ldots, N$.

Figure 3.2 demonstrates model (3.2.2). In this example, $r_0(\theta) = r_0$, so $f_1(\cdot)$ is a function of r_0, and $f_2(0, r_0, \mathbf{0}) = f_2(2\pi, r_0, \mathbf{0})$. Decomposition of deformation into lower and higher order terms reduces (3.2.2) to

$$\Delta r(\theta_i, r_0, \mathbf{0}) = c_{r_0} + \sum_k \{a_{r_0,k} \cos(k\theta_i) + b_{r_0,k} \sin(k\theta_i)\} + \epsilon_i, \tag{3.2.3}$$

where $f_1(r_0) = c_{r_0}$, and $\{a_{r_0,k},\ b_{r_0,k}\}$ are coefficients of a Fourier series expansion of $f_2(\cdot, \cdot, \mathbf{0})$. The $\{a_{r_0,k},\ b_{r_0,k}\}$ terms with large k represent the product's surface roughness, which is not of primary interest.

3.2.4 General Compensation and Interference Models

Under the polar coordinate system, a compensation of x_i units at θ_i can be thought of as an extension of the product's radius by x_i units in that specific direction. Bearing this in mind, we first follow Huang et al. (2013, p. 8) to extend (3.2.2) to accommodate compensations, and then build upon this work to give an extension that can help capture the interference that can result from discretized compensation plans.

Let $r(\theta_i, r_0(\cdot), (x_i, \ldots, x_i)) = r(\theta_i, r_0(\cdot), x_i)$ denote the potential radius for θ_i under application of x_i units of compensation to all points. Compensation of a product by x_i units at θ_i is equivalent, in terms of the final manufactured product, as if a CAD model with nominal radius $r_0(\cdot)+x_i$ and 0 compensation at θ_i was initially submitted to the 3D printer. Then

$$\begin{aligned} r(\theta_i, r_0(\cdot), x_i) - \{r_0(\theta_i) + x_i\} &= r(\theta_i, r_0(\cdot) + x_i, \mathbf{0}) - \{r_0(\theta_i) + x_i\} \\ &= \Delta r(\theta_i, r_0(\cdot) + x_i, \mathbf{0}), \end{aligned} \tag{*}$$

where $\Delta r(\theta_i, r_0(\cdot) + x_i, \mathbf{0})$ follows the same form as (3.2.2), abbreviated as

$$\Delta r(\theta_i, r_0(\cdot) + x_i, \mathbf{0}) = \mathbb{E}\{\Delta r(\theta_i, r_0(\cdot) + x_i, \mathbf{0})\} + \epsilon_i. \tag{**}$$

Consequently, the potential outcome for θ_i is

$$\begin{aligned}\Delta r(\theta_i, r_0(\cdot), x_i) &= r(\theta_i, r_0(\cdot), x_i) - r_0(\theta_i) \\ &= r(\theta_i, r_0(\cdot), x_i) - \{r_0(\theta_i) + x_i\} + x_i \\ &= \Delta r(\theta_i, r_0(\cdot) + x_i, \mathbf{0}) + x_i \\ &= \mathbb{E}\{\Delta r(\theta_i, r_0(\cdot) + x_i, \mathbf{0})\} + x_i + \epsilon_i. \end{aligned} \tag{3.2.4}$$

The last two steps follow from $(*)$ and $(**)$, respectively. If x_i is small relative to $r_0(\theta_i)$, then (3.2.4) can be approximated using the first and second terms of the Taylor expansion of $\mathbb{E}\{\Delta r(\theta_i, r_0(\cdot) + x_i, \mathbf{0})\}$ at $r_0(\theta_i)$:

$$\begin{aligned}\Delta r(\theta_i, r_0(\cdot), x_i) &\approx \mathbb{E}\{\Delta r(\theta_i, r_0(\cdot), \mathbf{0})\} \\ &\quad + (x_i - 0)\left[\frac{d}{dx}\mathbb{E}\{\Delta r(\theta_i, r_0(\cdot) + x, \mathbf{0})\}\right]_{x=0} + x_i + \epsilon_i \\ &= \Delta r(\theta_i, r_0(\cdot), \mathbf{0}) + \{1 + h(\theta_i, r_0(\cdot), \mathbf{0})\}x_i, \end{aligned} \tag{3.2.5}$$

where $h(\theta_i, r_0(\cdot), \mathbf{0}) = [d/dx\ \mathbb{E}\{\Delta r(\theta_i, r_0(\cdot) + x, \mathbf{0})\}]_{x=0}$. When a parametric model is specified for the potential outcomes, this Taylor expansion is performed conditional on the model parameters.

Although interference is not considered in (3.2.5), we can generalize this model to incorporate interference in a simple manner for a treatment assignment $\mathbf{x}$ with different units assigned different treatments. As all units are connected on the boundary of the product, unit θ_i's treatment effect will change due to interference from its neighbors. We believe that θ_i will deform not according to its assigned compensation x_i,

but instead according to a compensation $g_i(\mathbf{x})$ due to the proximity of neighboring units with different assigned compensations. Thus, we do not use only compensation x_i at θ_i to model the potential outcome for θ_i. Instead, we generalize (3.2.5) to

$$\Delta r(\theta_i, r_0(\cdot), \mathbf{x}) \approx \Delta r(\theta_i, r_0(\cdot), \mathbf{0}) + \{1 + h(\theta_i, r_0(\cdot), \mathbf{0})\} g_i(\mathbf{x}), \tag{3.2.6}$$

where the *effective treatment* $g_i(\mathbf{x})$ is a function of x_i and assigned compensations for neighbors of θ_i (with the definition of neighboring units naturally dependent on the specific product), hence potentially a function of the entire vector $\mathbf{x}$. This simple way to introduce interference, allowing the treatment effect for θ_i to depend on treatments assigned to its neighboring units, effectively incorporates interference in a meaningful manner, as will be seen in the analysis of our experiment.

3.3 Experimental Design and Analysis for Interference

3.3.1 Compensation Model for Cylinders

Huang et al. (2013, p. 12) constructed four cylinders with $r_0 = 0.5, 1, 2$, and 3 inches, and used $N_{0.5} = 749, N_1 = 707, N_2 = 700$, and $N_3 = 721$ equally-spaced units from each, displayed in Figure 3.3(a). Based on the logic in Section 3.2.3, they fitted

$$\Delta r(\theta_i, r_0, \mathbf{0}) = x_0 + \alpha(r_0 + x_0)^a + \beta(r_0 + x_0)^b \cos(2\theta_i) + \epsilon_i \tag{3.3.1}$$

to the data, with $\epsilon_i \sim \mathrm{N}(0, \sigma^2)$ independently, and parameters α, β, a, b, x_0, and σ independent of r_0. Specifically, for the cylinder, the location-independent term is thought to be proportional to r_0, so that under over exposure of x_0 units it would be of the form $x_0 + \alpha(r_0 + x_0)$. Furthermore, the location-dependent term should be a harmonic function of θ_i, and also proportional to r_0, of the form $\beta(r_0 + x_0)\cos(2\theta_i)$ under over exposure. Independent errors are used throughout because the focus is on a correct specification of the mean trend in deformation (Appendix C.1 contains a discussion on this point). Huang et al. (2013) specified

$$a \sim \mathrm{N}(1, 2^2),\ b \sim \mathrm{N}(1, 1^2),\ \log(x_0) \sim \mathrm{N}(0, 1^2),$$

and placed flat priors on α, β, and $\log(\sigma)$, with all parameters independent *a priori*. Posterior draws of the parameters were obtained by Hamiltonian Monte Carlo (HMC, Duane et al., 1987), and are summarized in Table 3.1, with convergence diagnostics discussed in Appendix C.2. A simple comparison of the posterior predictive distribution of product deformation to the observed data (Figure 3.3) demonstrates the good fit, and so we proceed with this specification and parameter inferences to design and analyze an experiment for interference.

Substituting $\Delta r(\theta_i, r_0, \mathbf{0})$ from (3.3.1) into the general model (3.2.4), we have

$$\Delta r(\theta_i, r_0, x_i) = x_0 + x_i + \alpha(r_0 + x_0 + x_i)^a + \beta(r_0 + x_0 + x_i)^b \cos(2\theta_i) + \epsilon_i. \quad (3.3.2)$$

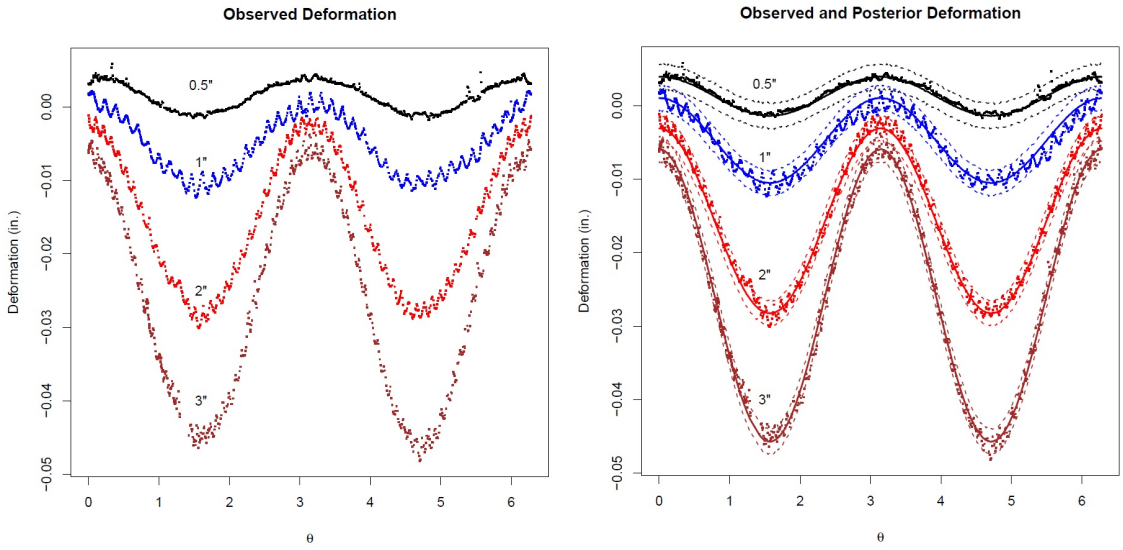

Figure 3.3: The left figure displays the observed deformation for $r_0 = 0.5, 1, 2$, and 3 inches, when no compensation is applied. The right figure displays a comparison of observed data with posterior predictions. Bold solid lines denote posterior means, and dashed lines the 2.5% and 97.5% posterior quantiles for each angle.

The Taylor expansion at $r_0 + x_0$, as in (3.2.5), yields the model

$$\Delta r(\theta_i, r_0, x_i) = x_0 + \alpha(r_0 + x_0)^a + \beta(r_0 + x_0)^b \cos(2\theta_i) + \left\{1 + a\alpha(r_0 + x_0)^{a-1} + b\beta(r_0 + x_0)^{b-1} \cos(2\theta_i)\right\} x_i + \epsilon_i. \quad (3.3.3)$$

We incorporate interference by changing x_i in (3.3.3) to $g_i(\mathbf{x})$, with the functional form of $g_i(\mathbf{x})$ derived by exploratory means in Section 3.3.3.

3.3.2 Experimental Design for Interference

Under a discretized compensation plan, the boundary of a product is divided into sections, with all points in one section assigned the same compensation. In the

Table 3.1: Summary of 1000 posterior draws of parameters after a burn-in of 500 when no compensation is applied. This is drawn from Table 5 in (Huang et al., 2013). Effective sample size is abbreviated as ESS throughout.

	Mean	SD	Median	95% Credible Interval	ESS
α	-1.34×10^{-2}	1.6×10^{-4}	-1.34×10^{-2}	$(-1.37, -1.31) \times 10^{-2}$	8198
β	5.7×10^{-3}	3.1×10^{-5}	5.71×10^{-3}	$(5.65, 5.8) \times 10^{-3}$	9522
a	8.61×10^{-1}	7.33×10^{-3}	8.61×10^{-1}	$(8.47, 8.75) \times 10^{-1}$	8223
b	1.13	5.46×10^{-3}	1.13	(1.12, 1.14)	9424
x_0	8.79×10^{-3}	1.5×10^{-4}	8.79×10^{-3}	$(8.5, 9.07) \times 10^{-3}$	8211
σ	8.7×10^{-4}	1.18×10^{-5}	8.7×10^{-4}	$(8.5, 8.9) \times 10^{-4}$	9384

terminology of Cox and Donnelly (2011, p. 18–19), these sections constitute units of analysis, and individual angles are units of interpretation. We expect interference for angles near neighboring sections. Interference should be substantial for a large difference in neighboring compensations, and negligible otherwise.

This reasoning led to the following restricted Latin square design to study interference. We apply compensations to four cylinders of radius $0.5, 1, 2$, and 3 inches, with each cylinder divided into 16 equal-sized sections of $\pi/8$ radians. One unit of compensation is $0.004, 0.008, 0.016$, and 0.03 inch for each respective cylinder, and there are only four possible levels of compensation, $-1, 0, +1$, and $+2$ units. Two blocking factors are considered. The first is the quadrant, and the second is the "symmetry group" consisting of $\pi/8$-radian sections that are reflections about the coordinate axes from each other. Symmetric sections form a meaningful block: if compensation x is applied to all units, then we have from (3.3.3) that for $0 \leq \theta \leq \pi/2$,

$$\begin{aligned}
\mathbb{E}\left\{\Delta r(\theta, r_0, x) \mid \alpha, \beta, a, b, x_0, \sigma\right\} &= \mathbb{E}\left\{\Delta r(\pi - \theta, r_0, x) \mid \alpha, \beta, a, b, x_0, \sigma\right\} \\
&= \mathbb{E}\left\{\Delta r(\pi + \theta, r_0, x) \mid \alpha, \beta, a, b, x_0, \sigma\right\} \\
&= \mathbb{E}\left\{\Delta r(2\pi - \theta, r_0, x) \mid \alpha, \beta, a, b, x_0, \sigma\right\},
\end{aligned}$$

suggesting a need to control for this symmetry in the experiment. Thus, for each product, we conceive of the 16 sections as a 4×4 table, with symmetry groups forming the column blocking factor, and quadrants the row blocking factor. Based on prior concerns about the possible severity of interference and resulting scope of inference from our model (3.2.5), the set of possible designs was restricted to Latin squares (each compensation level occurs only once in any quadrant and symmetry group), where the absolute difference in assigned treatments between two neighboring sections does not exceed two levels of compensation. Each product was randomly assigned one design from this set, with no further restriction that all the products have the same design.

Our restricted Latin square design forms a discretized compensation plan that blocks on two factors suggested by the previous deformaton model, and remains model-robust to a certain extent. The chosen experimental designs are in Figure 3.4, and observed deformations are in Figure 3.5. There are $N_{0.5} = 6159, N_1 = 6022, N_2 = 6206$, and $N_3 = 6056$ equally-spaced angles considered for the four cylinders.

3.3.3 Assessing the Structure of Interference

Our first task is to assess which units have negligible interference in the experiment. To do so, we use the suggestions of Sobel (2006) and Rosenbaum (2007), who describe when interest exists in comparing a treatment assignment $\mathbf{x}$ to a baseline.

We have in Section 3.3.1 data on cylinders that receive no compensation (denoted by $\mathbf{D}_n$), and a model (3.3.1) that provides a good fit. Furthermore, we have a hypothesized model (3.3.3) for compensation when interference is negligible, which is a

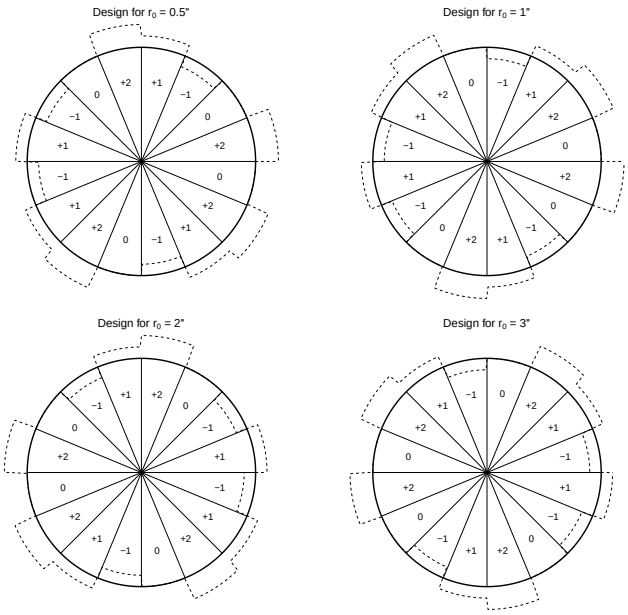

Figure 3.4: Experimental designs: dashed lines represent assigned compensations.

function of parameters in (3.3.1). If the manufacturing process is in control, posterior inferences based on $\mathbf{D}_n$ then yield, by (3.3.3), predictions for the experiment. In the absence of any other information, units in the experiment with observed outcomes deviating strongly from their predictions can be argued to have substantial interference. After all, if θ_i has negligible interference under assignment $\mathbf{x} = (x_1, \ldots, x_N)$, then

$$\Delta r(\theta_i, r_0, \mathbf{x}) = \Delta r(\theta_i, r_0, (x_i, \ldots, x_i)) = \Delta r(\theta_i, r_0, x_i).$$

This suggests the following procedure to assess interference:

1. Calculate the posterior distribution of the parameters conditional on $\mathbf{D}_n$, denoted by $\pi(\alpha, \beta, a, b, x_0, \sigma \mid \mathbf{D}_n)$.

2. For every angle in the four cylinders, form the posterior predictive distribution of the potential outcome corresponding to the observed treatment assignment

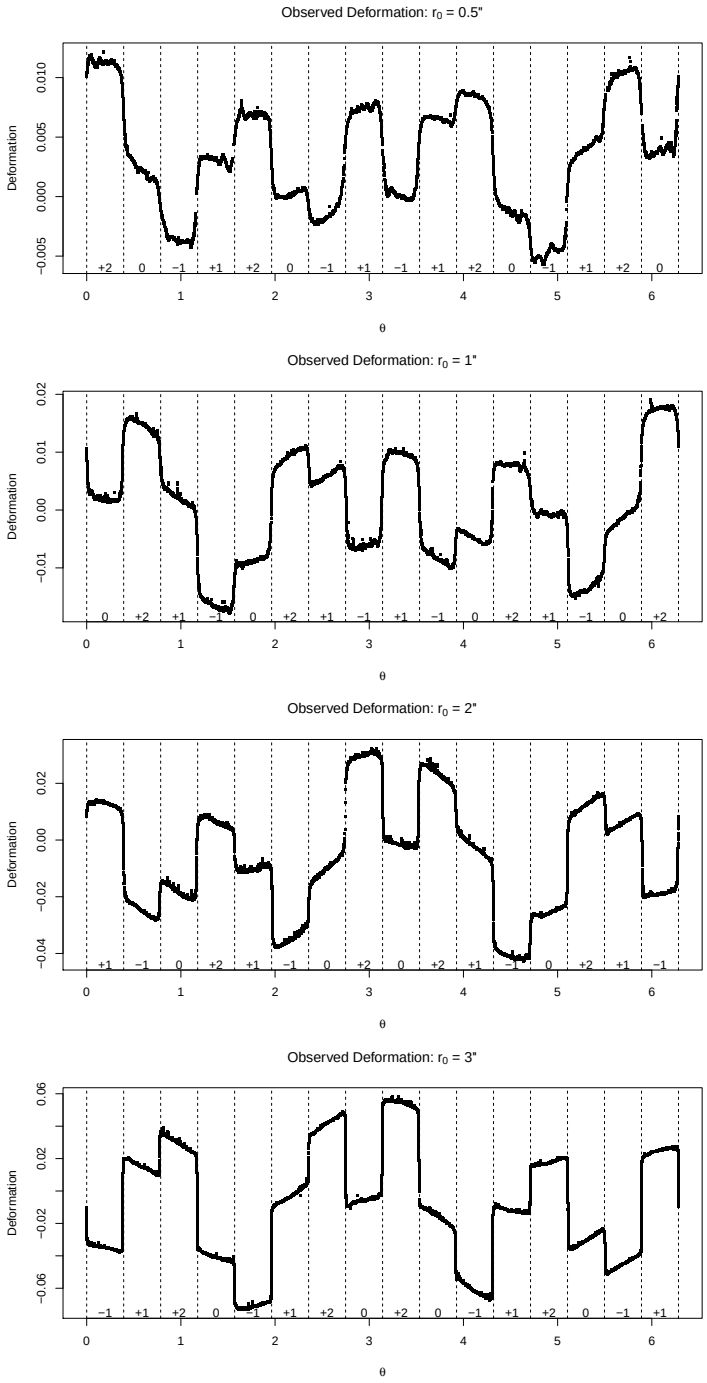

Figure 3.5: Observed deformations in the experiment. Dashed lines represent sections, and numbers at the bottom of each represent assigned compensations.

(Figure 3.4) using model (3.3.3) and $\pi(\alpha, \beta, a, b, x_0, \sigma \mid \mathbf{D}_n)$.

3. Compare the posterior predictive distributions to the observed deformations in the experiment.

   - If a unit's observed outcome falls within the 99% central posterior predictive interval and follows the posterior predictive mean trend, it is deemed to have negligible interference.
   - Otherwise, we conclude that the unit has substantial interference.

This procedure is similar to the construction of control charts (Box et al., 2009). When an observed outcome lies outside the 99% central posterior predictive interval, we suspect existence of a special cause. As the entire product is manufactured simultaneously, the only assignable cause is interference.

We implemented this procedure and observed that approximately $70\% - -80\%$ of units, primarily in the central regions of sections, have negligible interference (Appendix C.3). This is clearly seen with another graph that assesses effective treatments, which we proceed to describe.

Taking expectations in (3.3.3), the treatment effectively received by θ_i is

$$\frac{\mathbb{E}\left\{\Delta r(\theta_i, r_0, \mathbf{x}) \mid \alpha, \beta, a, b, x_0, \sigma\right\} - x_0 - \alpha(r_0 + x_0)^a - \beta(r_0 + x_0)^b \cos(2\theta_i)}{1 + a\alpha(r_0 + x_0)^{a-1} + b\beta(r_0 + x_0)^{b-1}\cos(2\theta_i)}. \tag{3.3.4}$$

We use (3.3.4) to gauge $g_i(\mathbf{x})$ by plugging observed data from the experiment and posterior draws of the parameters based on $\mathbf{D}_n$ into this equation. These discrepancy measure (Meng, 1994) calculations, summarized in Figure 3.6, again suggest that central angles in each section have negligible interference: estimates of their effective

treatments correspond to their assigned treatments. There is a slight discrepancy between assigned treatments and posterior predictive quantities for some central angles, but this is likely due to different parameter values for the two data sets. Of more importance is the observation that the effective treatment of a boundary angle θ_i is a weighted average of the treatment assigned to its section, $x_{i,M}$, and its nearest neighboring section, $x_{i,NM}$, with the weights a function of the distances (in radians) between θ_i and the midpoint angle of its section, $\theta_{i,M}$, and the midpoint angle of its nearest neighboring section, $\theta_{i,NM}$. All these observations correspond to the intuition that interference should be substantial near section boundaries.

3.3.4 A Simple Interference Model

We first alter (3.3.3) to

$$\begin{aligned}\Delta r(\theta_i, r_0, \mathbf{x}) = x_0 + \alpha(r_0 + x_0)^a + \beta(r_0 + x_0)^b \cos(2\theta_i) \\ + \left\{1 + a\alpha(r_0 + x_0)^{a-1} + b\beta(r_0 + x_0)^{b-1}\cos(2\theta_i)\right\} g_i(\mathbf{x}) + \epsilon_i, \quad (3.3.5)\end{aligned}$$

where

$$\begin{aligned}g_i(\mathbf{x}) = \left\{1 + \exp(-\lambda_{r_0}|\theta_i - \theta_{i,NM}| + \lambda_{r_0}|\theta_i - \theta_{i,M}|)\right\}^{-1} x_{i,M} \\ + \left\{1 + \exp(\lambda_{r_0}|\theta_i - \theta_{i,NM}| - \lambda_{r_0}|\theta_i - \theta_{i,M}|)\right\}^{-1} x_{i,NM}, \quad (3.3.6)\end{aligned}$$

with $\theta_{i,M}, \theta_{i,NM}$ denoting midpoint angles for the $\pi/8$-radian sections containing and neighboring nearest to θ_i, respectively, and $x_{i,M}, x_{i,NM}$ treatments assigned to these sections. Effective treatment $g_i(\mathbf{x})$ is a weighted average of the unit's assigned treat-

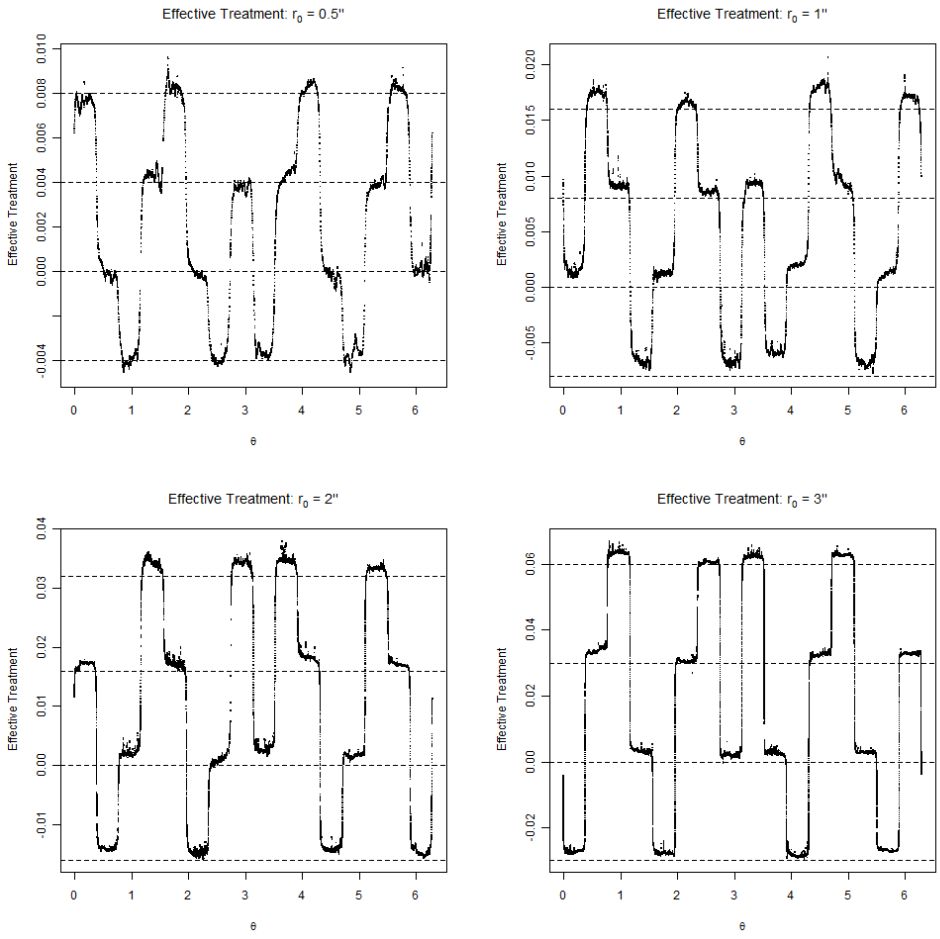

Figure 3.6: Gauging effective treatment $g_i(\mathbf{x})$ using (3.3.4). Four horizontal lines in each subfigure denote the possible compensations, and dots denote estimates of treatments that units effectively received in the experiment.

ment $x_i = x_{i,M}$ and the treatment $x_{i,NM}$ assigned to its nearest neighboring section. Although the form of the weights is chosen for computational convenience, we recognize that (3.3.6) belongs to a class of models agreeing with prior subject-matter knowledge that interference may be negligible if the implemented compensation is sufficiently "continuous", in the sense that the theoretical compensation plan is a continuous function of θ and the tolerance of the 3D printer is sufficiently fine so that discretization of compensation is negligible (Appendix C.4).

We fit the model in (3.3.5) and (3.3.6), having 10 total parameters, to the experiment data. The prior specification remains the same, with $\log(\lambda_{r_0}) \sim \mathrm{N}(0, 4^2)$ independently *a priori* for $r_0 = 0.5, 1, 2$, and 3 inches. A HMC algorithm was used to obtain 1000 draws from the joint posterior distribution after a burn-in of 500, and these are summarized in Table 3.2.

Table 3.2: Summary of posterior draws for simple interference model.

	Mean	SD	Median	95% Credible Interval	ESS
α	-1.06×10^{-2}	1.53×10^{-4}	-1.06×10^{-2}	$(-1.09, -1.03) \times 10^{-2}$	8078
β	5.79×10^{-3}	3.69×10^{-5}	5.79×10^{-3}	$(5.72, 5.86) \times 10^{-3}$	8237
a	9.5×10^{-1}	9.46×10^{-3}	9.5×10^{-1}	$(9.31, 9.69) \times 10^{-1}$	8150
b	1.12	6.64×10^{-3}	1.12	$(1.0, 1.13)$	8504
x_0	7.1×10^{-3}	1.43×10^{-4}	7.1×10^{-3}	$(6.82, 7.39) \times 10^{-3}$	8404
σ	3.14×10^{-3}	1.36×10^{-5}	3.14×10^{-3}	$(3.11, 3.17) \times 10^{-3}$	8924
$\lambda_{0.5}$	32.66	2.05	32.62	$(28.69, 36.76)$	8686
λ_1	48.24	2	48.12	$(44.5, 52.6)$	8666
λ_2	76.83	1.78	76.78	$(73.42, 80.44)$	8770
λ_3	86.08	0.83	86.06	$(84.49, 87.68)$	8385

This model provides a good fit for the 0.5 and 1 inch cylinders, but not the others. As an example, in Figure 3.7(a) the posterior mean trend does not correctly capture the observed transition across sections for the 3 inch cylinder. The problem appears to reside in (3.3.6). This specification implies that effective treatments of

units $\theta_i = k\pi/8$ for $k \in \mathbb{Z}_{>0}$ are equal-weighted averages of compensations applied to units $k\pi/8 \pm \pi/16$. To assess the validity of this implication, we use the posterior distribution of the parameters to calculate, for each θ_i, the inferred effective treatment in (3.3.4). An example of these calculations, Figure 3.7(b), shows that the inferred effective treatment for $\theta_i = \pi$ is nearly 0.06 inch, the compensation applied to its neighboring section. Thus, specification (3.3.6) is invalidated by the experiment.

Another posterior predictive check helps clarify the problem. From (3.3.6),

$$g_i(\mathbf{x}) = w_i x_{i,M} + (1 - w_i) x_{i,NM},$$

and so

$$w_i = \frac{g_i(\mathbf{x}) - x_{i,NM}}{x_{i,M} - x_{i,NM}}, \tag{3.3.7}$$

which is well-defined because $x_{i,M} \neq x_{i,NM}$ in this experiment. Plugging in the inferred effective treatments, calculated from (3.3.4), into (3.3.7), we then diagnose how to modify (3.3.6) to better model interference in the experiment.

This calculation was made for all cylinders, and the results for $r_0 = 3$ inches are summarized in Figure 3.8 as an example. Rows in this figure show the weights for each quadrant, and we focus on their behavior in neighborhoods of integral multiples of $\pi/8$. Neither the decay in the weights (represented by λ_{r_0} in (3.3.6)) nor the weight for integral multiples of $\pi/8$ remain constant across sections. In fact, these figures suggest that λ_{r_0} is a function of $\theta_{i,M}, \theta_{i,NM}$, and that a location term is required. They also demonstrate a possible subtle effect of quadrant, and as our experiment blocks on this factor, we are better able to use these posterior predictive checks to refine our

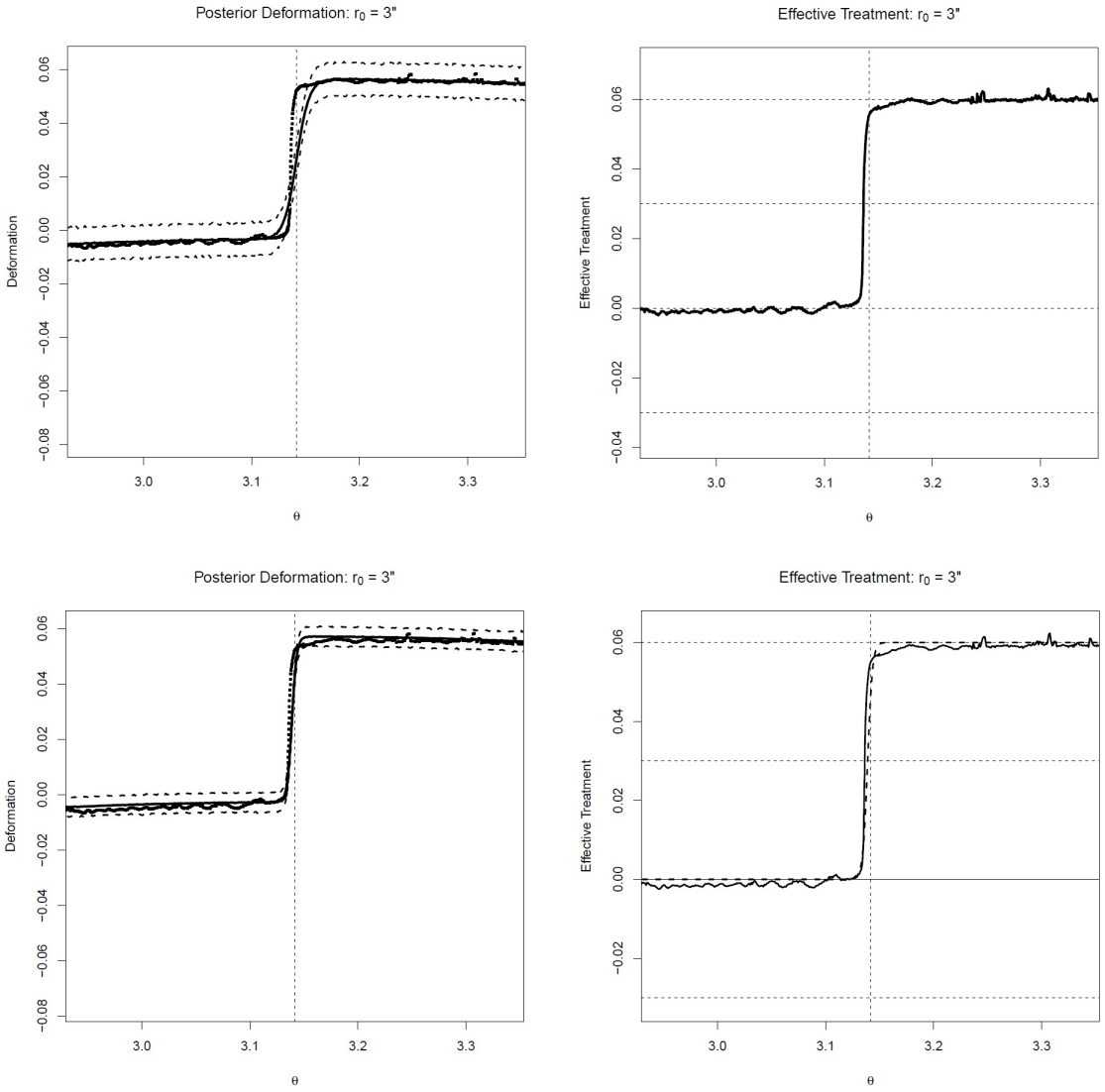

Figure 3.7: Counter-clockwise, from upper left: (a) An example of the type of erroneous predictions made by model (3.3.5), (3.3.6) for the 3 inch cylinder. The vertical line is drawn at $\theta = \pi$, marking the boundary between two sections. Units to the left of this line were given 0 compensation, and units to the right were given +2 compensation. The posterior mean trend is represented by the solid line, and posterior quantiles are represented by dashed lines. Observed data are denoted by dots. (b): Corresponding inferred effective treatment for $15\pi/16 \leq \theta \leq 17\pi/16$. (c): Refined posterior predictions for $r_0 = 3''$, $15\pi/16 \leq \theta \leq 17\pi/16$. (d): Comparing inferred effective treatments (solid line) with refined effective treatment model (dashed-line) for the 3 inch cylinder.

simple interference model and capture this unexpected pattern in deformation across quadrants.

3.3.5 A Refined Interference Model

Our refined effective treatment model is of the same functional form as (3.3.6), with λ_{r_0} replaced by $\lambda_{r_0}(\theta_{i,M}, \theta_{i,NM})$, and $|\theta_i - \theta_{i,M}|, |\theta_i - \theta_{i,NM}|$ replaced by $|\theta_i - \theta_{i,M} - \delta_{r_0}(\theta_{i,M}, \theta_{i,NM})|, |\theta_i - \theta_{i,NM} - \delta_{r_0}(\theta_{i,M}, \theta_{i,NM})|$, respectively. Here, $\delta_{r_0}(\theta_{i,M}, \theta_{i,NM})$ represent location shifts across sections suggested by our posterior predictive checks.

Our specific model is

$$\delta_{r_0}(\theta_{i,M}, \theta_{i,NM}) = \delta_{r_0,0} + \sum_{k=1}^{3} \left\{ \delta^c_{r_0,k} \cos(k\theta_{i,B}) + \delta^s_{r_0,k} \sin(k\theta_{i,B}) \right\}, \tag{3.3.8}$$

$$\lambda_{r_0}(\theta_{i,M}, \theta_{i,NM}) = \mathbb{I}(|x_{i,M} - x_{i,NM}| = 1)\lambda_{r_0,1} + \mathbb{I}(|x_{i,M} - x_{i,NM}| = 2)\lambda_{r_0,2}, \tag{3.3.9}$$

where $\theta_{i,B} = (\theta_{i,M} + \theta_{i,NM})/2$ and $|x_{i,M} - x_{i,NM}|$ is measured in absolute units of compensation here. From Figure 3.8 and the fact that

$$\delta_{r_0}(\theta_{i,M}, \theta_{i,NM}) = \delta_{r_0}(\theta_{i,M} + 2\pi, \theta_{i,NM} + 2\pi),$$

location shifts should be modeled using harmonic functions.

This model provides a better fit. Comparing Figure 3.7(c), which displays posterior predictions from the refined model (based on one chain of posterior draws using a standard random walk Metropolis algorithm), with the previous model's predictions in Figure 3.7(a), we immediately see that the refined model better captures the

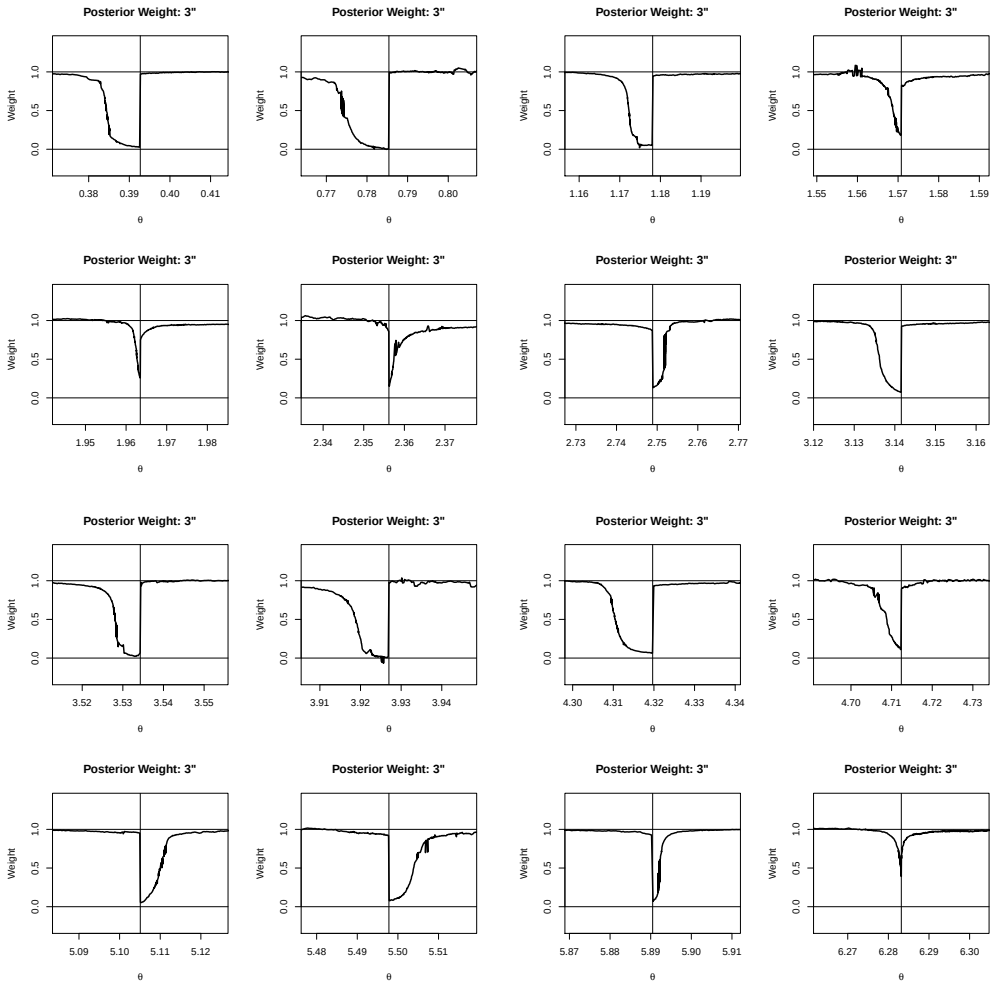

Figure 3.8: Inferring weights in the interference model for the $r_0 = 3$ inch cylinder, using effective treatments calculated from equation (3.3.4) based on the posterior distribution of parameters from Section 3.3.4. Vertical lines are drawn at $\theta = k\pi/8$ for $k = 1, \ldots, 16$.

posterior mean trend. Similar improvements exist for the other sections and cylinders. We also compare the original inferred effective treatments obtained from (3.3.4) with the refined model in Figure 3.7(d) and see that the new model better captures interference.

3.3.6 Summary of the Experimental Design and Analysis

Three key ingredients relating to the data, model, and experimental design have made our series of analyses possible, and are relevant and useful across a wide variety of disciplines. First is the availability of benchmark data, e.g., every unit on the cylinder receiving zero compensation. Second is the potential outcomes model (3.3.3) for the effect of compensation, defined in terms of a fixed number of parameters that do not depend on the vector of treatment assignments $\mathbf{x}$. These two enable calculation of the posterior predictive distribution of potential outcomes under the assumption of negligible interference. The final ingredient is the explicit distinction between units of analysis and units of interpretation in our design, which provides the means to assess and model interference in the experiment. Comparing observed outcomes from the experiment to posterior predictions allows one to infer the structure of interference, which can be validated by further experimentation.

These considerations suggest that our methodology can be generalized and applied to other experimental situations with units residing on connected surfaces. In general, when experimenting with units on a connected surface, a principled and step-by-step analysis using the three ingredients above, as illustrated in this paper, can ultimately shed more light on the substantive question of interest.

3.4 Conclusion: Ignoring Interference Inhibits Improvements

To construct 3D printed products satisfying manufacturing demands on dimensional accuracy, it is important to address the problem of interference in a principled manner. Huang et al. (2013) recognized that continuous compensation plans implemented on printers with a sufficiently fine tolerance can effectively control a product's printed dimensions without inducing additional complications through interference. Their models for product deformation motivated our experiment that introduces interference through the application of a discretized compensation plan to the boundary of a cylinder. Combining this experiment's data with inferences based on data for which every unit received no compensation led to an assessment of interference in terms of how units' effective treatments differed from that physically assigned. Further analyses effectively modeled interference in the experiment.

It is important to note that the refined interference model's location and scale terms (3.3.8), (3.3.9) are a function of the compensation plan. For example, reflecting the assigned compensations across the y axis would accordingly change the location shifts. The implication of this and all our previous observations for manufacturing is that severely discretized compensation plans introduce interference, and if this fact is ignored, then dimensional accuracy control for 3D printed products will be hindered, especially for geometrically complex products relevant in real-life manufacturing.

It is worthwhile to note that there is an interesting connection between interference modeling and the classic robust design approach (Taguchi, 1987) for dimensional

accuracy control in 3D printing. As pointed out by several authors, e.g., Wu and Hamada (2009, Ch. 11) and Dasgupta and Wu (2006), response function modeling is a useful step in any robust design problem, when the response is modeled as a function of control and noise factors, and a suitable performance measure (e.g., the signal-to-noise ratio) is derived from the fitted response function. The principle of robust design can successfully be applied only if the response model contains interaction terms between the control factors and the noise factors. In our current context, as before, let x_i denote the compensation applied to the ith unit, and $\mathbf{x}_i^-$ the compensations applied to all other units. Then obtaining an optimal or "robust" compensation entails the following two steps: (i) expressing the deformation as a function $\Delta r(\theta_i, r_0(\cdot), x_i, \mathbf{x}_i^-)$, and (ii) choosing $\mathbf{x}$ such that a performance measure of unit-level deformation is minimized. Our focus on understanding interference between units can also be viewed as identifying significant interactions between x_i and $\mathbf{x}_i^-$ and fitting an appropriate response function model, which is nothing but response function modeling in the robust design context. The question of robustness only arises if such interactions exist.

Many research challenges and opportunities for both statistics and additive manufacturing remain to be addressed. Perhaps the most important is experimental design in the presence of interference. For example, when focus is on construction of specific classes of products (e.g., complicated gear structures), optimum designs can lead to precise estimates of model parameters, hence improved compensation plans and control of deformation. An important and subtle statistical issue that then arises is how the structure of interference changes as a function of the compensation plan derived

from the experimental design. Instead of being a weighted average of the treatment applied to its section and nearest neighboring section, the derived compensation plan may cause a unit's effective treatment to be a weighted average of treatments applied to other sections as well, with weights depending on the absolute difference in applied compensations. Knowledge of the relationship between compensation plans derived from specific experimental designs and interference is necessary to improve dimensional accuracy control in general, and therefore is an important issue to address for 3D printing.

Appendix A

Supplementary Materials for Chapter 1

This supplement contains our reworking of Neyman's calculations. It is important to note that, although our proofs may not be technically elegant, they are designed to reveal explicitly the errors of Neyman (1935).

A.1 Randomized Complete Block Designs

Consider N blocks and T treatments, with each block having T experimental units, and treatments randomized to experimental units independently across blocks. We define

$$W_{ij}(t) = \begin{cases} 1 & \text{if unit } j \text{ in block } i \text{ is assigned treatment } t, \\ 0 & \text{otherwise.} \end{cases}$$

Following Neyman (1935), the potential outcome of unit $j = 1, \ldots, T$ in block $i = 1, \ldots, N$ under treatment $t = 1, \ldots, T$ is

$$x_{ij}(t) = X_{ij}(t) + \epsilon_{ij}(t),$$

where $X_{ij}(t) \in \mathbb{R}$ is an unknown constant and $\epsilon_{ij}(t) \sim [0, \sigma_\epsilon^2]$ are iid and independent of treatment indicators $\mathbf{W} = \{W_{ij}(t)\}$. The potential outcomes are decomposed into

$$x_{ij}(t) = \bar{X}_{\cdot\cdot}(t) + B_i(t) + \eta_{ij}(t) + \epsilon_{ij}(t),$$

where

$$B_i(t) = \bar{X}_{i\cdot}(t) - \bar{X}_{\cdot\cdot}(t),$$

$$\eta_{ij}(t) = X_{ij}(t) - \bar{X}_{i\cdot}(t).$$

Define $y_i(t)$ as the observed response of the unit assigned treatment t in block i,

$$y_i(t) = \sum_{j=1}^{T} W_{ij}(t) x_{ij}(t),$$

and $\bar{y}_{\cdot}(t)$ as the observed average response for units assigned treatment t,

$$\bar{y}_{\cdot}(t) = \frac{1}{N} \sum_{i=1}^{N} y_i(t).$$

We see that

$$\mathbb{E}\{\bar{y}_{\cdot}(t)\} = \mathbb{E}[\mathbb{E}\{\bar{y}_{\cdot}(t)|\mathbf{W}\}] = \mathbb{E}\left\{\frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{T} W_{ij}(t) X_{ij}(t)\right\} = \bar{X}_{\cdot\cdot}(t),$$

so $\bar{y}_{\cdot}(t) - \bar{y}_{\cdot}(t')$ is unbiased for $\bar{X}_{\cdot\cdot}(t) - \bar{X}_{\cdot\cdot}(t')$. We proceed to calculate the variance of this statistic as

$$\mathrm{Var}\{\bar{y}_{\cdot}(t) - \bar{y}_{\cdot}(t')\} = \frac{2\sigma_\epsilon^2 + \sigma_\eta^2(t) + \sigma_\eta^2(t')}{N} + \frac{2r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')}}{N(T-1)},$$

where we define

$$\sigma_\eta^2(t) = \frac{1}{NT}\sum_{i=1}^{N}\sum_{j=1}^{T}\eta_{ij}(t)^2,$$

$$r(t,t') = \frac{\sum_{i=1}^{N}\sum_{j=1}^{T}\eta_{ij}(t)\eta_{ij}(t')}{NT\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')}}.$$

First, we calculate $\mathrm{Var}\{\bar{y}_{\cdot}(t)\} = \{\sigma_\epsilon^2 + \sigma_\eta^2(t)\}/N$. Note that for $j \neq j',\ i \neq i'$,

$$\mathrm{Cov}\{W_{ij}(t), W_{ij'}(t)\} = \mathbb{E}\{W_{ij}(t)W_{ij'}(t)\} - \mathbb{E}\{W_{ij}(t)\}\mathbb{E}\{W_{ij'}(t)\} = -\frac{1}{T^2},$$

$$\mathrm{Cov}\{W_{ij}(t), W_{i'j}(t)\} = \mathrm{Cov}\{W_{ij}(t), W_{i'j'}(t)\} = 0.$$

Then

$$\begin{aligned}
\mathrm{Var}\{\bar{y}_{\cdot}(t)\} &= \mathbb{E}[\mathrm{Var}\{\bar{y}_{\cdot}(t)|\mathbf{W}\}] + \mathrm{Var}[\mathbb{E}\{\bar{y}_{\cdot}(t)|\mathbf{W}\}] \\
&= \mathbb{E}\left\{\frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{T} W_{ij}(t)^2\sigma_\epsilon^2\right\} \\
&\quad + \mathrm{Var}\left[\frac{1}{N}\sum_{i=1}^{N}\sum_{j=1}^{T} W_{ij}(t)\{\bar{X}_{\cdot\cdot}(t) + B_i(t) + \eta_{ij}(t)\}\right] \\
&= \frac{\sigma_\epsilon^2}{N} + \frac{1}{N^2}\sum_{i=1}^{N}\mathrm{Var}\left\{\sum_{j=1}^{T} W_{ij}(t)\eta_{ij}(t)\right\} \\
&= \frac{\sigma_\epsilon^2}{N} + \frac{1}{N^2}\sum_{i=1}^{N}\left\{\sum_{j=1}^{T}\frac{1}{T}\left(1-\frac{1}{T}\right)\eta_{ij}(t)^2 + \sum_{j\neq j'}\left(-\frac{1}{T^2}\right)\eta_{ij}(t)\eta_{ij'}(t)\right\} \\
&= \frac{\sigma_\epsilon^2}{N} + \frac{1}{N^2T}\sum_{i=1}^{N}\sum_{j=1}^{T}\eta_{ij}(t)^2 - \frac{1}{N^2T^2}\sum_{i=1}^{N}\left\{\sum_{j=1}^{T}\eta_{ij}(t)\right\}^2 \\
&= \frac{\sigma_\epsilon^2 + \sigma_\eta^2(t)}{N}.
\end{aligned}$$

To find $\mathrm{Cov}\{\bar{y}_{\cdot}(t), \bar{y}_{\cdot}(t')\} = -r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')}/\{N(T-1)\}$, note that

$$\mathrm{Cov}\{\bar{y}_{\cdot}(t), \bar{y}_{\cdot}(t')|\mathbf{W}\} = \frac{1}{N^2}\mathrm{Cov}\left\{\sum_{i=1}^{N}\sum_{j=1}^{T} W_{ij}(t)\epsilon_{ij}(t), \sum_{i=1}^{N}\sum_{j=1}^{T} W_{ij}(t')\epsilon_{ij}(t')|\mathbf{W}\right\} = 0,$$

$$\begin{aligned}
\mathbb{E}\{\bar{y}_{\cdot}(t)|\mathbf{W}\} &= \frac{1}{N}\sum_{i=1}^{N}\sum_{j=1}^{T} W_{ij}(t)\{\bar{X}_{\cdot\cdot}(t) + B_i(t) + \eta_{ij}(t)\} \\
&= \bar{X}_{\cdot\cdot}(t) + \frac{1}{N}\sum_{i=1}^{N}\sum_{j=1}^{T} W_{ij}(t)\eta_{ij}(t).
\end{aligned}$$

Then

$$\begin{aligned}
\mathrm{Cov}\{\bar{y}_{\cdot}(t), \bar{y}_{\cdot}(t')\} &= \mathbb{E}[\mathrm{Cov}\{\bar{y}_{\cdot}(t), \bar{y}_{\cdot}(t')|\mathbf{W}\}] + \mathrm{Cov}[\mathbb{E}\{\bar{y}_{\cdot}(t)|\mathbf{W}\}, \mathbb{E}\{\bar{y}_{\cdot}(t')|\mathbf{W}\}] \\
&= \frac{1}{N^2}\mathrm{Cov}\left\{\sum_{i=1}^{N}\sum_{j=1}^{T} W_{ij}(t)\eta_{ij}(t), \sum_{i=1}^{N}\sum_{j=1}^{T} W_{ij}(t')\eta_{ij}(t')\right\} \\
&= \frac{1}{N^2}\sum_{i=1}^{N}\mathrm{Cov}\left\{\sum_{j=1}^{T} W_{ij}(t)\eta_{ij}(t), \sum_{j=1}^{T} W_{ij}(t')\eta_{ij}(t')\right\} \\
&= \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{T}\left(-\frac{1}{T^2}\right)\eta_{ij}(t)\eta_{ij}(t') \\
&\quad + \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j\neq j'}\left\{\frac{1}{T(T-1)} - \frac{1}{T^2}\right\}\eta_{ij}(t)\eta_{ij'}(t') \\
&= -\frac{r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')}}{N(T-1)}.
\end{aligned}$$

Thus

$$\mathrm{Var}\{\bar{y}_{\cdot}(t) - \bar{y}_{\cdot}(t')\} = \frac{2\sigma_\epsilon^2 + \sigma_\eta^2(t) + \sigma_\eta^2(t')}{N} + \frac{2r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')}}{N(T-1)}.$$

We now calculate expectations of sums of squares, starting with residual sum of squares

$$(N-1)(T-1)S_0^2 = \sum_{i=1}^{N}\sum_{t=1}^{T}\{y_i(t) - \bar{y}_{\cdot}(t) - \bar{y}_i(\cdot) + \bar{y}_{\cdot}(\cdot)\}^2,$$

where we rewrite

$$\{y_i(t)-\bar{y}_{\cdot}(t)-\bar{y}_i(\cdot)+\bar{y}_{\cdot}(\cdot)\}^2 = \{y_i(t)-\bar{y}_{\cdot}(t)\}^2+\{\bar{y}_i(\cdot)-\bar{y}_{\cdot}(\cdot)\}^2-2\{y_i(t)-\bar{y}_{\cdot}(t)\}\{\bar{y}_i(\cdot)-\bar{y}_{\cdot}(\cdot)\}.$$

As

$$\mathbb{E}\{y_i(t) - \bar{y}_{\cdot}(t)\} = \frac{1}{T}\sum_{j=1}^{T} X_{ij}(t) - \frac{1}{NT}\sum_{i=1}^{N}\sum_{j=1}^{T} X_{ij}(t) = B_i(t),$$

we have

$$\mathbb{E}\{y_i(t) - \bar{y}_\cdot(t)\}^2 = \mathrm{Var}\{y_i(t)\} + \mathrm{Var}\{\bar{y}_\cdot(t)\} - 2\mathrm{Cov}\{y_i(t), \bar{y}_\cdot(t)\} + B_i(t)^2.$$

Also,

$$\begin{aligned}\mathrm{Var}\{y_i(t)\} &= \mathbb{E}\left\{\sum_{j=1}^{T} W_{ij}(t)^2\sigma_\epsilon^2\right\} + \mathrm{Var}\left[\sum_{j=1}^{T} W_{ij}(t)\{\bar{X}_{\cdot\cdot}(t) + B_i(t) + \eta_{ij}(t)\}\right] \\ &= \sigma_\epsilon^2 + \frac{1}{T}\sum_{j=1}^{T}\eta_{ij}(t)^2.\end{aligned}$$

For now, we write

$$\mathbb{E}\{y_i(t) - \bar{y}_\cdot(t)\}^2 = \sigma_\epsilon^2 + \frac{1}{T}\sum_{j=1}^{T}\eta_{ij}(t)^2 + \frac{\sigma_\epsilon^2 + \sigma_\eta^2(t)}{N} - 2\mathrm{Cov}\{y_i(t), \bar{y}_\cdot(t)\} + B_i(t)^2.$$

From above,

$$\mathbb{E}\{\bar{y}_i(\cdot) - \bar{y}_\cdot(\cdot)\} = \frac{1}{T}\sum_{t=1}^{T}\mathbb{E}\{y_i(t) - \bar{y}_\cdot(t)\} = \bar{B}_i(\cdot),$$

and we write

$$\mathbb{E}\{\bar{y}_i(\cdot) - \bar{y}_\cdot(\cdot)\}^2 = \mathrm{Var}\{\bar{y}_i(\cdot)\} + \mathrm{Var}\{\bar{y}_\cdot(\cdot)\} - 2\mathrm{Cov}\{\bar{y}_i(\cdot), \bar{y}_\cdot(\cdot)\} + \bar{B}_i(\cdot)^2.$$

Finally,

$$\begin{aligned}\mathbb{E}[\{y_i(t) - \bar{y}_\cdot(t)\}\{\bar{y}_i(\cdot) - \bar{y}_\cdot(\cdot)\}] = \mathrm{Cov}\{y_i(t), \bar{y}_i(\cdot)\} - \mathrm{Cov}\{y_i(t), \bar{y}_\cdot(\cdot)\} \\ - \mathrm{Cov}\{\bar{y}_\cdot(t), \bar{y}_i(\cdot)\} + \mathrm{Cov}\{\bar{y}_\cdot(t), \bar{y}_\cdot(\cdot)\} \\ + B_i(t)\bar{B}_i(\cdot).\end{aligned}$$

To simplify remaining calculations, we evaluate $\mathrm{Cov}\{y_i(t), y_i(t')\}$ and $\mathrm{Var}\{\bar{y}_\cdot(\cdot)\}$.

$$\begin{aligned}\mathrm{Cov}\{y_i(t), y_i(t')\} &= \mathrm{Cov}\left\{\sum_{j=1}^{T} W_{ij}(t)X_{ij}(t), \sum_{j=1}^{T} W_{ij}(t')X_{ij}(t')\right\} \\ &= \mathrm{Cov}\left\{\sum_{j=1}^{T} W_{ij}(t)\eta_{ij}(t), \sum_{j=1}^{T} W_{ij}(t')\eta_{ij}(t')\right\} \\ &= \sum_{j=1}^{T} \mathrm{Cov}\{W_{ij}(t)\eta_{ij}(t), W_{ij}(t')\eta_{ij}(t')\} \\ &\quad + \sum_{j\neq j'} \mathrm{Cov}\{W_{ij}(t)\eta_{ij}(t), W_{ij'}(t')\eta_{ij'}(t')\} \\ &= -\frac{1}{T^2}\sum_{j=1}^{T} \eta_{ij}(t)\eta_{ij}(t') + \left\{\frac{1}{T(T-1)} - \frac{1}{T^2}\right\}\sum_{j\neq j'} \eta_{ij}(t)\eta_{ij'}(t') \\ &= -\frac{1}{T(T-1)}\sum_{j=1}^{T} \eta_{ij}(t)\eta_{ij}(t') \\ &\quad + \left\{\frac{1}{T(T-1)} - \frac{1}{T^2}\right\}\left\{\sum_{j=1}^{T} \eta_{ij}(t)\right\}\left\{\sum_{j=1}^{T} \eta_{ij}(t')\right\} \\ &= -\frac{1}{T(T-1)}\sum_{j=1}^{T} \eta_{ij}(t)\eta_{ij}(t').\end{aligned}$$

As treatments are assigned independently across blocks,

$$\begin{aligned}
\mathrm{Var}\{\bar{y}_{\cdot}(\cdot)\} &= \frac{1}{N^2}\sum_{i=1}^{N}\mathrm{Var}\{\bar{y}_i(\cdot)\} \\
&= \left(\frac{1}{NT}\right)^2\sum_{i=1}^{N}\left[\sum_{t=1}^{T}\mathrm{Var}\{y_i(t)\}+\sum_{t\neq t'}\mathrm{Cov}\{y_i(t),y_i(t')\}\right] \\
&= \left(\frac{1}{NT}\right)^2\sum_{i=1}^{N}\sum_{t=1}^{T}\left\{\sigma_\epsilon^2+\frac{1}{T}\sum_{j=1}^{T}\eta_{ij}(t)^2\right\} \\
&\quad -\left(\frac{1}{NT}\right)^2\sum_{i=1}^{N}\left\{\frac{1}{T(T-1)}\sum_{t\neq t'}\sum_{j=1}^{T}\eta_{ij}(t)\eta_{ij}(t')\right\} \\
&= \left(\frac{1}{NT}\right)^2\left\{NT\sigma_\epsilon^2+\frac{1}{T}\sum_{i=1}^{N}\sum_{j=1}^{T}\sum_{t=1}^{T}\eta_{ij}(t)^2\right\} \\
&\quad -\left(\frac{1}{NT}\right)^2\left\{\frac{1}{T(T-1)}\sum_{t\neq t'}\sum_{i=1}^{N}\sum_{j=1}^{T}\eta_{ij}(t)\eta_{ij}(t')\right\} \\
&= \frac{\sigma_\epsilon^2}{NT}+\frac{1}{NT^2}\sum_{t=1}^{T}\sigma_\eta^2(t)-\frac{1}{NT^2(T-1)}\sum_{t\neq t'}r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')}.
\end{aligned}$$

Finally, we note that

$$\sum_{i=1}^{N}\sum_{t=1}^{T}\{B_i(t)^2-\bar{B}_i(\cdot)^2\}=\sum_{i=1}^{N}\sum_{t=1}^{T}\{B_i(t)-\bar{B}_i(\cdot)\}^2.$$

We use all these results for the following simplifications:

$$\begin{aligned}
\sum_{i=1}^{N}\sum_{t=1}^{T}\mathbb{E}\{y_i(t)-\bar{y}_{\cdot}(t)\}^2 &= (N+1)T\sigma_\epsilon^2+(N+1)\sum_{t=1}^{T}\sigma_\eta^2(t)-2N\sum_{t=1}^{T}\mathrm{Var}\{\bar{y}_{\cdot}(t)\} \\
&\quad +\sum_{i=1}^{N}\sum_{t=1}^{T}B_i(t)^2,
\end{aligned}$$

$$\sum_{i=1}^{N}\sum_{t=1}^{T}\mathbb{E}\{\bar{y}_i(\cdot)-\bar{y}_\cdot(\cdot)\}^2 = N(N-1)T\mathrm{Var}\{\bar{y}_\cdot(\cdot)\}+\sum_{i=1}^{N}\sum_{t=1}^{T}\bar{B}_i(\cdot)^2,$$

$$-2\sum_{i=1}^{N}\sum_{t=1}^{T}\mathbb{E}[\{y_i(t)-\bar{y}_\cdot(t)\}\{\bar{y}_i(\cdot)-\bar{y}_\cdot(\cdot)\}] = -2N(N-1)T\mathrm{Var}\{\bar{y}_\cdot(\cdot)\}-2\sum_{i=1}^{N}\sum_{t=1}^{T}\bar{B}_i(\cdot)^2.$$

Combining these terms, we obtain

$$\begin{aligned}\mathbb{E}\{(N-1)(T-1)S_0^2\} &= (N+1)T\sigma_\epsilon^2+(N+1)\sum_{t=1}^{T}\sigma_\eta^2(t)-N(N-1)T\mathrm{Var}\{\bar{y}_\cdot(\cdot)\}\\ &\quad -2N\sum_{t=1}^{T}\mathrm{Var}\{\bar{y}_\cdot(t)\}+\sum_{i=1}^{N}\sum_{t=1}^{T}\{B_i(t)^2-\bar{B}_i(\cdot)^2\}\\ &= (N-1)T\sigma_\epsilon^2+(N-1)\sum_{t=1}^{T}\sigma_\eta^2(t)-N(N-1)T\mathrm{Var}\{\bar{y}_\cdot(\cdot)\}\\ &\quad +\sum_{i=1}^{N}\sum_{t=1}^{T}\{B_i(t)-\bar{B}_i(\cdot)\}^2,\end{aligned}$$

so that

$$\begin{aligned}\mathbb{E}\{(N-1)(T-1)S_0^2\} &= (N-1)(T-1)\sigma_\epsilon^2+(N-1)\left(1-\frac{1}{T}\right)\sum_{t=1}^{T}\sigma_\eta^2(t)\\ &\quad +\frac{N-1}{T(T-1)}\sum_{t\neq t'}r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')}\\ &\quad +\sum_{i=1}^{N}\sum_{t=1}^{T}\{B_i(t)-\bar{B}_i(\cdot)\}^2.\end{aligned}$$

This is the correct expression for the expected residual sum of squares. As

$$\sum_{i=1}^{N}\sum_{t=1}^{T}\{B_i(t)-\bar{B}_i(\cdot)\}^2\neq 0$$

in general, this differs from the one given by Neyman, which we ow derive.

From pages 147-148 of his appendix, we see that Neyman calculates

$$\mathbb{E}\{(N-1)(T-1)S_0^2\} = (N-1)(T-1)\mathbb{E}(S_0'^2 + S_0''^2),$$

where we define

$$S_0'^2 = \sum_{i=1}^{N}\sum_{t=1}^{T}\{\eta_i(t) - \bar{\eta}_\cdot(t) - \bar{\eta}_i(\cdot) + \bar{\eta}_\cdot(\cdot)\}^2,$$

$$S_0''^2 = \sum_{i=1}^{N}\sum_{t=1}^{T}\{\epsilon_i(t) - \bar{\epsilon}_\cdot(t) - \bar{\epsilon}_i(\cdot) + \bar{\epsilon}_\cdot(\cdot)\}^2,$$

$$\eta_i(t) = \sum_{j=1}^{T} W_{ij}(t)\eta_{ij}(t), \quad \epsilon_i(t) = \sum_{j=1}^{T} W_{ij}(t)\epsilon_{ij}(t).$$

We have from equations $(21) - (24)$ in Neyman's appendix that

$$\begin{aligned}\mathbb{E}\left\{(N-1)(T-1)\sum_{i=1}^{N}\sum_{t=1}^{T}\eta_i(t)^2\right\} &= \frac{(N-1)(T-1)}{T}\sum_{i=1}^{N}\sum_{j=1}^{T}\sum_{t=1}^{T}\eta_{ij}(t)^2 \\ &= N(N-1)(T-1)\sum_{t=1}^{T}\sigma_\eta^2(t),\end{aligned}$$

$$\begin{aligned}\mathbb{E}\left\{-(N-1)\sum_{t\neq t'}\sum_{i=1}^{N}\eta_i(t)\eta_i(t')\right\} &= -\frac{N-1}{T(T-1)}\sum_{t\neq t'}\sum_{i=1}^{N}\sum_{j\neq j'}\eta_{ij}(t)\eta_{ij'}(t') \\ &= \frac{N-1}{T(T-1)}\sum_{t\neq t'}\sum_{i=1}^{N}\sum_{j=1}^{T}\eta_{ij}(t)\eta_{ij}(t') \\ &\quad - \frac{N-1}{T(T-1)}\sum_{t\neq t'}\sum_{i=1}^{N}\left\{\sum_{j=1}^{T}\eta_{ij}(t)\right\}\left\{\sum_{j=1}^{T}\eta_{ij}(t')\right\} \\ &= \frac{N(N-1)}{T-1}\sum_{t\neq t'} r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')}.\end{aligned}$$

Using Neyman's notation

$$\mathbb{E}(S_0'^2) = \frac{1}{T}\sum_{t=1}^{T}\sigma_\eta^2(t) + \frac{1}{T(T-1)^2}\sum_{t\neq t'} r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')},$$

$$\mathbb{E}(S_0''^2) = \sigma_\epsilon^2.$$

Thus, Neyman obtains

$$\mathbb{E}(S_0^2) = \sigma_\epsilon^2 + \frac{1}{T}\sum_{t=1}^{T}\sigma_\eta^2(t) + \frac{1}{T(T-1)^2}\sum_{t\neq t} r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')}.$$

We see that Neyman's result for the expected mean residual sum of squares is generally less than the correct expression. In fact, Neyman's error occurs in equation (17) on page 147 of his appendix. His final result is missing the term $\sum_{i=1}^{N}\sum_{t=1}^{T}\{B_i(t) - \bar{B}_i(\cdot)\}^2/\{(N-1)(T-1)\}$.

We finally calculate the expectation of the mean treatment sum of squares,

$$S_1^2 = \frac{N}{T-1}\sum_{t=1}^{T}\left\{\bar{y}_\cdot(t) - \bar{y}_\cdot(\cdot)\right\}^2.$$

Now $\mathbb{E}\{\bar{y}_{\cdot}(t)\} = \bar{X}_{\cdot\cdot}(t),\ \mathbb{E}\{\bar{y}_{\cdot}(\cdot)\} = \bar{X}_{\cdot\cdot}(\cdot)$, so that

$$\begin{aligned}
\mathbb{E}(S_1^2) &= \frac{N}{T-1}\sum_{t=1}^{T}\left[\mathrm{Var}\{\bar{y}_{\cdot}(t)\} + \mathrm{Var}\{\bar{y}_{\cdot}(\cdot)\} - 2\mathrm{Cov}\{\bar{y}_{\cdot}(t), \bar{y}_{\cdot}(\cdot)\} + \{\bar{X}_{\cdot\cdot}(t) - \bar{X}_{\cdot\cdot}(\cdot)\}^2\right] \\
&= \frac{N}{T-1}\left[\sum_{t=1}^{T}\mathrm{Var}\{\bar{y}_{\cdot}(t)\} + T\mathrm{Var}\{\bar{y}_{\cdot}(\cdot)\} - 2T\mathrm{Var}\{\bar{y}_{\cdot}(\cdot)\} + \sum_{t=1}^{T}\{\bar{X}_{\cdot\cdot}(t) - \bar{X}_{\cdot\cdot}(\cdot)\}^2\right] \\
&= \sigma_\epsilon^2 + \frac{1}{T}\sum_{t=1}^{T}\sigma_\eta^2(t) + \frac{1}{T(T-1)^2}\sum_{t\neq t'} r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')} \\
&\quad + \frac{N}{T-1}\sum_{t=1}^{T}\{\bar{X}_{\cdot\cdot}(t) - \bar{X}_{\cdot\cdot}(\cdot)\}^2,
\end{aligned}$$

which corresponds to Neyman's result.

A.2 Latin Square Designs

We now consider $T \times T$ LSs, with rows and columns denoting levels of two blocking factors. Define

$$W_{ij}(t) = \begin{cases} 1 & \text{if the unit in row } i,\ \text{column } j,\ \text{is assigned treatment } t, \\ 0 & \text{otherwise.} \end{cases}$$

The potential outcome of unit (i, j) under treatment t is

$$x_{ij}(t) = X_{ij}(t) + \epsilon_{ij}(t),$$

with $X_{ij}(t) \in \mathbb{R}$ an unknown constant and $\epsilon_{ij}(t) \sim [0, \sigma_\epsilon^2]$ iid and independent of the $W_{ij}(t)$. These are decomposed into

$$x_{ij}(t) = \bar{X}_{\cdot\cdot}(t) + R_i(t) + C_j(t) + \eta_{ij}(t) + \epsilon_{ij}(t),$$

where

$$R_i(t) = \bar{X}_{i\cdot}(t) - \bar{X}_{\cdot\cdot}(t),$$

$$C_j(t) = \bar{X}_{\cdot j}(t) - \bar{X}_{\cdot\cdot}(t),$$

$$\eta_{ij}(t) = X_{ij}(t) - \bar{X}_{i\cdot}(t) - \bar{X}_{\cdot j}(t) + \bar{X}_{\cdot\cdot}(t).$$

Define $\bar{x}^o_{\cdot\cdot}(t)$ as the observed average response for units assigned treatment t,

$$\bar{x}^o_{\cdot\cdot}(t) = \frac{1}{T}\sum_{i=1}^{T}\sum_{j=1}^{T} W_{ij}(t)x_{ij}(t).$$

To calculate expectations for the LS, we use the following probabilities, which are proven in the next subsection:

$$\Pr\{W_{ij}(t) = 1\} = \frac{1}{T},$$

$$\Pr\{W_{ij}(t) = W_{ij'}(t) = 1\} = \Pr\{W_{ij}(t) = W_{i'j}(t) = 1\} = 0,$$

$$\begin{aligned}\Pr\{W_{ij}(t) = W_{ij'}(t') = 1\} &= \Pr\{W_{ij}(t) = W_{i'j}(t') = 1\} \\ &= \Pr\{W_{ij}(t) = W_{i'j'}(t) = 1\} \\ &= \frac{1}{T(T-1)},\end{aligned}$$

$$\Pr\{W_{ij}(t) = W_{i'j'}(t') = 1\} = \frac{T-2}{T(T-1)^2}.$$

Again, $\mathbb{E}\{\bar{x}^o_{\cdot\cdot}(t)\} = \bar{X}_{\cdot\cdot}(t)$. We next calculate $\mathrm{Var}\{\bar{x}^o_{\cdot\cdot}(t)\} = \sigma^2_\epsilon/T + \sigma^2_\eta(t)/(T-1)$, where

$$\sigma^2_\eta(t) = \frac{1}{T^2}\sum_{i=1}^{T}\sum_{j=1}^{T}\eta_{ij}(t)^2.$$

As $\sum_{i=1}^{T} R_i(t) = \sum_{j=1}^{T} C_j(t) = 0$ and $\sum_{i=1}^{T} W_{ij}(t) = \sum_{j=1}^{T} W_{ij}(t) = 1$,

$$\bar{x}^o_{\cdot\cdot}(t) = \bar{X}_{\cdot\cdot}(t) + \frac{1}{T}\sum_{i=1}^{T}\sum_{j=1}^{T} W_{ij}(t)\eta_{ij}(t) + \frac{1}{T}\sum_{i=1}^{T}\sum_{j=1}^{T} W_{ij}(t)\epsilon_{ij}(t).$$

By conditioning on $\mathbf{W}$,

$$\begin{aligned}\mathrm{Var}\{\bar{x}^o_{\cdot\cdot}(t)\} &= \mathbb{E}\left\{\frac{\sigma^2_\epsilon}{T^2}\sum_{i=1}^{T}\sum_{j=1}^{T} W_{ij}(t)^2\right\} + \mathrm{Var}\left\{\frac{1}{T}\sum_{i=1}^{T}\sum_{j=1}^{T} W_{ij}(t)\eta_{ij}(t)\right\} \\ &= \frac{\sigma^2_\epsilon}{T} + \frac{1}{T^2}\mathrm{Var}\left\{\sum_{i=1}^{T}\sum_{j=1}^{T} W_{ij}(t)\eta_{ij}(t)\right\}.\end{aligned}$$

We see that

$$\begin{aligned}
\mathrm{Var}\left\{\sum_{i=1}^{T}\sum_{j=1}^{T} W_{ij}(t)\eta_{ij}(t)\right\} &= \sum_{i=1}^{T}\sum_{j=1}^{T}\left(\frac{1}{T}-\frac{1}{T^2}\right)\eta_{ij}(t)^2 \\
&\quad + \sum_{i=1}^{T}\sum_{j\neq j'}\left(-\frac{1}{T^2}\right)\eta_{ij}(t)\eta_{ij'}(t) \\
&\quad + \sum_{i\neq i'}\sum_{j=1}^{T}\left(-\frac{1}{T^2}\right)\eta_{ij}(t)\eta_{i'j}(t) \\
&\quad + \sum_{i\neq i'}\sum_{j\neq j'}\left\{\frac{1}{T(T-1)}-\frac{1}{T^2}\right\}\eta_{ij}(t)\eta_{i'j'}(t) \\
&= \frac{1}{T}\sum_{i=1}^{T}\sum_{j=1}^{T}\eta_{ij}(t)^2 - \frac{1}{T^2}\left\{\sum_{i=1}^{T}\sum_{j=1}^{T}\eta_{ij}(t)\right\}^2 \\
&\quad + \frac{1}{T(T-1)}\sum_{i\neq i'}\sum_{j\neq j'}\eta_{ij}(t)\eta_{i'j'}(t).
\end{aligned}$$

Now $\sum_{i=1}^{T}\eta_{ij}(t) = \sum_{j=1}^{T}\eta_{ij}(t) = 0$, and for fixed $i, j \in \{1,\ldots,T\}$,

$$\sum_{i'\neq i}\sum_{j'\neq j}\eta_{ij}(t)\eta_{i'j'}(t) = \eta_{ij}(t)\sum_{i'\neq i}\sum_{j'\neq j}\eta_{i'j'}(t) = \eta_{ij}(t)\sum_{i'\neq i}\{-\eta_{i'j}(t)\} = \eta_{ij}(t)^2.$$

Hence

$$\begin{aligned}
\mathrm{Var}\left\{\sum_{i=1}^{T}\sum_{j=1}^{T} W_{ij}(t)\eta_{ij}(t)\right\} &= \left\{\frac{1}{T}+\frac{1}{T(T-1)}\right\}\sum_{i=1}^{T}\sum_{j=1}^{T}\eta_{ij}(t)^2 \\
&= \frac{1}{T-1}\sum_{i=1}^{T}\sum_{j=1}^{T}\eta_{ij}(t)^2,
\end{aligned}$$

and so $\mathrm{Var}\{\bar{x}^{o}_{\cdot\cdot}(t)\} = \sigma_\epsilon^2/T + \sigma_\eta^2(t)/(T-1)$.

We now calculate $\text{Cov}\{\bar{x}^o_{\cdot\cdot}(t), \bar{x}^o_{\cdot\cdot}(t')\} = -r(t,t')\sqrt{\sigma^2_\eta(t)\sigma^2_\eta(t')}/(T-1)^2$, where

$$r(t,t') = \frac{\sum_{i=1}^T \sum_{j=1}^T \eta_{ij}(t)\eta_{ij}(t')}{T^2\sqrt{\sigma^2_\eta(t)\sigma^2_\eta(t')}}.$$

We see that

$$\text{Cov}\{\bar{x}^o_{\cdot\cdot}(t), \bar{x}^o_{\cdot\cdot}(t')|\mathbf{W}\} = \frac{1}{T^2}\text{Cov}\left\{\sum_{i=1}^T\sum_{j=1}^T W_{ij}(t)\epsilon_{ij}(t), \sum_{i=1}^T\sum_{j=1}^T W_{ij}(t')\epsilon_{ij}(t')|\mathbf{W}\right\} = 0,$$

$$\mathbb{E}\{\bar{x}^o_{\cdot\cdot}(t)|\mathbf{W}\} = \bar{X}_{\cdot\cdot}(t) + \frac{1}{T}\sum_{i=1}^T\sum_{j=1}^T W_{ij}(t)\eta_{ij}(t),$$

$$\begin{aligned}
\text{Cov}[\mathbb{E}\{\bar{x}^o_{\cdot\cdot}(t)|\mathbf{W}\}, \mathbb{E}\{\bar{x}^o_{\cdot\cdot}(t')|\mathbf{W}\}] &= \frac{1}{T^2}\text{Cov}\left\{\sum_{i=1}^T\sum_{j=1}^T W_{ij}(t)\eta_{ij}(t), \sum_{i=1}^T\sum_{j=1}^T W_{ij}(t')\eta_{ij}(t')\right\} \\
&= \frac{1}{T^2}\sum_{i=1}^T\sum_{j=1}^T\left(-\frac{1}{T^2}\right)\eta_{ij}(t)\eta_{ij}(t') \\
&\quad + \frac{1}{T^2}\sum_{i=1}^T\sum_{j\neq j'}\left\{\frac{1}{T(T-1)} - \frac{1}{T^2}\right\}\eta_{ij}(t)\eta_{ij'}(t') \\
&\quad + \frac{1}{T^2}\sum_{i\neq i'}\sum_{j=1}^T\left\{\frac{1}{T(T-1)} - \frac{1}{T^2}\right\}\eta_{ij}(t)\eta_{i'j}(t') \\
&\quad + \frac{1}{T^2}\sum_{i\neq i'}\sum_{j\neq j'}\left\{\frac{T-2}{T(T-1)^2} - \frac{1}{T^2}\right\}\eta_{ij}(t)\eta_{i'j'}(t') \\
&= -\frac{1}{T^4}\left\{\sum_{i=1}^T\sum_{j=1}^T\eta_{ij}(t)\right\}\left\{\sum_{i=1}^T\sum_{j=1}^T\eta_{ij}(t')\right\} \\
&\quad - \frac{1}{T^2(T-1)^2}\sum_{i=1}^T\sum_{j=1}^T\eta_{ij}(t)\eta_{ij}(t') \\
&= -\frac{r(t,t')\sqrt{\sigma^2_\eta(t)\sigma^2_\eta(t')}}{(T-1)^2}.
\end{aligned}$$

We have from all these calculations that

$$\mathrm{Var}\{\bar{x}^o_{\cdot\cdot}(t) - \bar{x}^o_{\cdot\cdot}(t')\} = \frac{2\sigma^2_\epsilon}{T} + \frac{\sigma^2_\eta(t) + \sigma^2_\eta(t')}{T-1} + \frac{2r(t,t')\sqrt{\sigma^2_\eta(t)\sigma^2_\eta(t')}}{(T-1)^2}.$$

The residual and treatment sums of squares are (respectively)

$$(T-1)(T-2)S_0^2 = \sum_{i=1}^T \sum_{j=1}^T \left\{ y_{ij} - \bar{y}_{i\cdot} - \bar{y}_{\cdot j} - \sum_{t=1}^T W_{ij}(t)\bar{x}^o_{\cdot\cdot}(t) + 2\bar{y}_{\cdot\cdot} \right\}^2,$$

$$(T-1)S_1^2 = T\sum_{t=1}^T \{\bar{x}^o_{\cdot\cdot}(t) - \bar{y}_{\cdot\cdot}\}^2,$$

where $y_{ij} = \sum_{t=1}^T W_{ij}(t)x_{ij}(t)$ is the observed response of cell (i,j) and

$$\bar{y}_{i\cdot} = \frac{1}{T}\sum_{j=1}^T y_{ij}, \quad \bar{y}_{\cdot j} = \frac{1}{T}\sum_{i=1}^T y_{ij}, \quad \bar{y}_{\cdot\cdot} = \frac{1}{T}\sum_{j=1}^T \bar{y}_{\cdot j} = \frac{1}{T}\sum_{i=1}^T \bar{y}_{i\cdot} = \frac{1}{T^2}\sum_{i=1}^T\sum_{j=1}^T y_{ij}.$$

We calculate the expected residual sum of squares by subtracting the sum of the expected treatment, column, and row sums of squares from the expected total sum of squares. We see that

$$\begin{aligned}
\mathbb{E}\left\{ \sum_{i=1}^T\sum_{j=1}^T (y_{ij} - \bar{y}_{\cdot\cdot})^2 \right\} &= \sum_{i=1}^T\sum_{j=1}^T \mathrm{Var}(y_{ij} - \bar{y}_{\cdot\cdot}) + \sum_{i=1}^T\sum_{j=1}^T \{\bar{X}_{ij}(\cdot) - \bar{X}_{\cdot\cdot}(\cdot)\}^2 \\
&= \sum_{i=1}^T\sum_{j=1}^T \mathrm{Var}(y_{ij}) - T^2\mathrm{Var}(\bar{y}_{\cdot\cdot}) + \sum_{i=1}^T\sum_{j=1}^T \{\bar{X}_{ij}(\cdot) - \bar{X}_{\cdot\cdot}(\cdot)\}^2,
\end{aligned}$$

$$\mathbb{E}\left[T\sum_{t=1}^{T}\{\bar{x}^{o}_{\cdot\cdot}(t)-\bar{y}_{\cdot\cdot}\}^2\right] = T\sum_{t=1}^{T}\mathrm{Var}\{\bar{x}^{o}_{\cdot\cdot}(t)-\bar{y}_{\cdot\cdot}\}+T\sum_{t=1}^{T}\{\bar{X}_{\cdot\cdot}(t)-\bar{X}_{\cdot\cdot}(\cdot)\}^2$$
$$= T\sum_{t=1}^{T}\mathrm{Var}\{\bar{x}^{o}_{\cdot\cdot}(t)\}-T^2\mathrm{Var}(\bar{y}_{\cdot\cdot})+T\sum_{t=1}^{T}\{\bar{X}_{\cdot\cdot}(t)-\bar{X}_{\cdot\cdot}(\cdot)\}^2,$$

$$\mathbb{E}\left\{T\sum_{j=1}^{T}(\bar{y}_{\cdot j}-\bar{y}_{\cdot\cdot})^2\right\} = T\sum_{j=1}^{T}\mathrm{Var}(\bar{y}_{\cdot j}-\bar{y}_{\cdot\cdot})+T\sum_{j=1}^{T}\{\bar{X}_{\cdot j}(\cdot)-\bar{X}_{\cdot\cdot}(\cdot)\}^2$$
$$= T\sum_{j=1}^{T}\mathrm{Var}(\bar{y}_{\cdot j})-T^2\mathrm{Var}(\bar{y}_{\cdot\cdot})+T\sum_{j=1}^{T}\{\bar{X}_{\cdot j}(\cdot)-\bar{X}_{\cdot\cdot}(\cdot)\}^2,$$

$$\mathbb{E}\left\{T\sum_{i=1}^{T}(\bar{y}_{i\cdot}-\bar{y}_{\cdot\cdot})^2\right\} = T\sum_{i=1}^{T}\mathrm{Var}(\bar{y}_{i\cdot}-\bar{y}_{\cdot\cdot})+T\sum_{i=1}^{T}\{\bar{X}_{i\cdot}(\cdot)-\bar{X}_{\cdot\cdot}(\cdot)\}^2$$
$$= T\sum_{i=1}^{T}\mathrm{Var}(\bar{y}_{i\cdot})-T^2\mathrm{Var}(\bar{y}_{\cdot\cdot})+T\sum_{i=1}^{T}\{\bar{X}_{i\cdot}(\cdot)-\bar{X}_{\cdot\cdot}(\cdot)\}^2.$$

The expected residual sum of squares is the sum of

$$\sum_{i=1}^{T}\sum_{j=1}^{T}\mathrm{Var}(y_{ij})-T\sum_{t=1}^{T}\mathrm{Var}\{\bar{x}^{o}_{\cdot\cdot}(t)\}, \tag{A.2.1}$$

$$-T\left\{\sum_{i=1}^{T}\mathrm{Var}(\bar{y}_{i\cdot})+\sum_{j=1}^{T}\mathrm{Var}(\bar{y}_{\cdot j})-2T\mathrm{Var}(\bar{y}_{\cdot\cdot})\right\}, \tag{A.2.2}$$

$$\frac{1}{T}\sum_{i=1}^{T}\sum_{j=1}^{T}\sum_{t=1}^{T}[\{\bar{X}_{ij}(\cdot)-\bar{X}_{\cdot\cdot}(\cdot)\}^2-\{\bar{X}_{\cdot\cdot}(t)-\bar{X}_{\cdot\cdot}(\cdot)\}^2-\{\bar{X}_{\cdot j}(\cdot)-\bar{X}_{\cdot\cdot}(\cdot)\}^2$$
$$-\{\bar{X}_{i\cdot}(\cdot)-\bar{X}_{\cdot\cdot}(\cdot)\}^2], \tag{A.2.3}$$

and we proceed to evaluate each of these three terms.

First note that (by conditioning on $\mathbf{W}$),

$$\begin{aligned}
\mathrm{Var}(y_{ij}) &= \sigma_\epsilon^2 + \mathrm{Var}\left\{\sum_{t=1}^{T} W_{ij}(t)X_{ij}(t)\right\} \\
&= \sigma_\epsilon^2 + \sum_{t=1}^{T}\left(\frac{1}{T} - \frac{1}{T^2}\right)X_{ij}(t)^2 + \sum_{t\neq t'}\left(-\frac{1}{T^2}\right)X_{ij}(t)X_{ij}(t') \\
&= \sigma_\epsilon^2 + \frac{1}{T}\sum_{t=1}^{T} X_{ij}(t)^2 - \bar{X}_{ij}(\cdot)^2 \\
&= \sigma_\epsilon^2 + \frac{1}{T}\sum_{t=1}^{T}\left\{X_{ij}(t) - \bar{X}_{ij}(\cdot)\right\}^2.
\end{aligned}$$

As such, (A.2.1) can be written as

$$T(T-1)\sigma_\epsilon^2 + \frac{1}{T}\sum_{i=1}^{T}\sum_{j=1}^{T}\sum_{t=1}^{T}\{X_{ij}(t) - \bar{X}_{ij}(\cdot)\}^2 - \frac{T}{T-1}\sum_{t=1}^{T}\sigma_\eta^2(t),$$

which we expand as

$$\begin{aligned}
T(T-1)\sigma_\epsilon^2 &+ T\sum_{t=1}^{T}\{\bar{X}_{\cdot\cdot}(t) - \bar{X}_{\cdot\cdot}(\cdot)\}^2 + \sum_{i=1}^{T}\sum_{t=1}^{T}\{R_i(t) - \bar{R}_i(\cdot)\}^2 \\
&+ \sum_{j=1}^{T}\sum_{t=1}^{T}\{C_j(t) - \bar{C}_j(\cdot)\}^2 + \frac{1}{T}\sum_{i=1}^{T}\sum_{j=1}^{T}\sum_{t=1}^{T}\{\eta_{ij}(t) - \bar{\eta}_{ij}(\cdot)\}^2 \\
&- \frac{T}{T-1}\sum_{t=1}^{T}\sigma_\eta^2(t).
\end{aligned}$$

To write out the expression for (A.2.2), note that

$$\mathrm{Var}(\bar{y}_{\cdot\cdot}) = \mathrm{Var}\left\{\frac{1}{T}\sum_{t=1}^{T}\bar{x}_{\cdot\cdot}^{o}(t)\right\} = \frac{1}{T^2}\sum_{t=1}^{T}\mathrm{Var}\{\bar{x}_{\cdot\cdot}^{o}(t)\} + \frac{1}{T^2}\sum_{t\neq t'}\mathrm{Cov}\{\bar{x}_{\cdot\cdot}^{o}(t), \bar{x}_{\cdot\cdot}^{o}(t')\},$$

and so

$$2T^2\mathrm{Var}(\bar{y}_{\cdot\cdot}) = 2\sigma_\epsilon^2 + \frac{2}{T-1}\sum_{t=1}^{T}\sigma_\eta^2(t) - \frac{2}{(T-1)^2}\sum_{t\neq t'} r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')}.$$

By conditioning on $\mathbf{W}$, we have

$$\begin{aligned}
\mathrm{Cov}(y_{ij}, y_{ij'}) &= -\frac{1}{T(T-1)}\sum_{t=1}^{T} X_{ij}(t)X_{ij'}(t) + \left(\frac{1}{T-1}\right)\bar{X}_{ij}(\cdot)\bar{X}_{ij'}(\cdot), \\
\mathrm{Cov}(y_{ij}, y_{i'j}) &= -\frac{1}{T(T-1)}\sum_{t=1}^{T} X_{ij}(t)X_{i'j}(t) + \left(\frac{1}{T-1}\right)\bar{X}_{ij}(\cdot)\bar{X}_{i'j}(\cdot).
\end{aligned}$$

With these relations in mind,

$$\begin{aligned}
-T\sum_{i=1}^{T}\mathrm{Var}(\bar{y}_{i\cdot}) &= -\frac{1}{T}\sum_{i=1}^{T}\sum_{j=1}^{T}\mathrm{Var}(y_{ij}) - \frac{1}{T}\sum_{i=1}^{T}\sum_{j\neq j'}\mathrm{Cov}(y_{ij}, y_{ij'}) \\
&= -\frac{1}{T}\sum_{i=1}^{T}\sum_{j=1}^{T}\left[\sigma_\epsilon^2 + \frac{1}{T}\sum_{t=1}^{T}\{X_{ij}(t) - \bar{X}_{ij}(\cdot)\}^2\right] \\
&\quad + \frac{1}{T^2(T-1)}\sum_{i=1}^{T}\sum_{j\neq j'}\left\{\sum_{t=1}^{T} X_{ij}(t)X_{ij'}(t) - T\bar{X}_{ij}(\cdot)\bar{X}_{ij'}(\cdot)\right\},
\end{aligned}$$

and

$$\sum_{i=1}^{T}\sum_{j\neq j'}\left\{\sum_{t=1}^{T} X_{ij}(t)X_{ij'}(t)\right\} = \sum_{i=1}^{T}\sum_{j=1}^{T}\sum_{t=1}^{T} X_{ij}(t)\{T\bar{X}_{i\cdot}(t) - X_{ij}(t)\},$$

$$\sum_{i=1}^{T}\sum_{j\neq j'}\{-T\bar{X}_{ij}(\cdot)\bar{X}_{ij'}(\cdot)\} = -\sum_{i=1}^{T}\sum_{j=1}^{T} T\bar{X}_{ij}(\cdot)\{T\bar{X}_{i\cdot}(\cdot) - \bar{X}_{ij}(\cdot)\}.$$

By symmetry,

$$
\begin{aligned}
-T\sum_{j=1}^{T}\mathrm{Var}(\bar{y}_{\cdot j}) &= -\frac{1}{T}\sum_{j=1}^{T}\sum_{i=1}^{T}\mathrm{Var}(y_{ij}) - \frac{1}{T}\sum_{j=1}^{T}\sum_{i\neq i'}\mathrm{Cov}(y_{ij}, y_{i'j}) \\
&= -\frac{1}{T}\sum_{j=1}^{T}\sum_{i=1}^{T}\left[\sigma_\epsilon^2 + \frac{1}{T}\sum_{t=1}^{T}\{X_{ij}(t) - \bar{X}_{ij}(\cdot)\}^2\right] \\
&\quad + \frac{1}{T^2(T-1)}\sum_{j=1}^{T}\sum_{i\neq i'}\left\{\sum_{t=1}^{T}X_{ij}(t)X_{i'j}(t) - T\bar{X}_{ij}(\cdot)\bar{X}_{i'j}(\cdot)\right\},
\end{aligned}
$$

and

$$
\sum_{j=1}^{T}\sum_{i\neq i'}\left\{\sum_{t=1}^{T}X_{ij}(t)X_{i'j}(t)\right\} = \sum_{i=1}^{T}\sum_{j=1}^{T}\sum_{t=1}^{T}X_{ij}(t)\{T\bar{X}_{\cdot j}(t) - X_{ij}(t)\},
$$

$$
\sum_{j=1}^{T}\sum_{i\neq i'}\{-T\bar{X}_{ij}(\cdot)\bar{X}_{i'j}(\cdot)\} = -\sum_{i=1}^{T}\sum_{j=1}^{T}T\bar{X}_{ij}(\cdot)\{T\bar{X}_{\cdot j}(\cdot) - \bar{X}_{ij}(\cdot)\}.
$$

By combining all these terms, we have that (A.2.2) equals

$$
\begin{aligned}
&-2(T-1)\sigma_\epsilon^2 - \frac{2}{T(T-1)}\sum_{i=1}^{T}\sum_{j=1}^{T}\sum_{t=1}^{T}\{X_{ij}(t) - \bar{X}_{ij}(\cdot)\}^2 \\
&\quad + \frac{1}{T-1}\sum_{i=1}^{T}\sum_{t=1}^{T}\{\bar{X}_{i\cdot}(t) - \bar{X}_{i\cdot}(\cdot)\}^2 + \frac{1}{T-1}\sum_{j=1}^{T}\sum_{t=1}^{T}\{\bar{X}_{\cdot j}(t) - \bar{X}_{\cdot j}(\cdot)\}^2 \\
&\quad + \frac{2}{T-1}\sum_{t=1}^{T}\sigma_\eta^2(t) - \frac{2}{(T-1)^2}\sum_{t\neq t'}r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')}.
\end{aligned}
$$

We rewrite this expression to obtain

$$
\begin{aligned}
&- 2(T-1)\sigma_\epsilon^2 + \frac{2}{T-1}\sum_{t=1}^{T}\sigma_\eta^2(t) - \frac{2}{(T-1)^2}\sum_{t\neq t'} r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')} \\
&- \frac{1}{T-1}\left[\sum_{i=1}^{T}\sum_{t=1}^{T}\{R_i(t) - \bar{R}_i(\cdot)\}^2 + \sum_{j=1}^{T}\sum_{t=1}^{T}\{C_j(t) - \bar{C}_j(\cdot)\}^2\right] \\
&- \frac{1}{T-1}\left[\frac{2}{T}\sum_{i=1}^{T}\sum_{j=1}^{T}\sum_{t=1}^{T}\{\eta_{ij}(t) - \bar{\eta}_{ij}(\cdot)\}^2\right].
\end{aligned}
$$

To finish with the third term, we note that

$$
\bar{X}_{ij}(\cdot) = \bar{X}_{i\cdot}(\cdot) + \bar{X}_{\cdot j}(\cdot) + \bar{\eta}_{ij}(\cdot) - \bar{X}_{\cdot\cdot}(\cdot),
$$

so that

$$
\begin{aligned}
\sum_{i=1}^{T}\sum_{j=1}^{T}\{\bar{X}_{ij}(\cdot) - \bar{X}_{\cdot\cdot}(\cdot)\}^2 = T\sum_{i=1}^{T}\{\bar{X}_{i\cdot}(\cdot) - \bar{X}_{\cdot\cdot}(\cdot)\}^2 + T\sum_{j=1}^{T}\{\bar{X}_{\cdot j}(\cdot) - \bar{X}_{\cdot\cdot}(\cdot)\}^2 \\
+ \sum_{i=1}^{T}\sum_{j=1}^{T}\bar{\eta}_{ij}(\cdot)^2.
\end{aligned}
$$

Hence, we write (A.2.3) as

$$
\sum_{t=1}^{T}\sigma_\eta^2(t) + \sum_{t\neq t'} r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')} - T\sum_{t=1}^{T}\{\bar{X}_{\cdot\cdot}(t) - \bar{X}_{\cdot\cdot}(\cdot)\}^2.
$$

We add all these three terms to obtain (after algebraic simplification)

$$\begin{aligned}\mathbb{E}\{(T-1)(T-2)S_0^2\} &= (T-1)(T-2)\sigma_\epsilon^2 + \frac{(T-2)^2}{T-1}\sum_{t=1}^{T}\sigma_\eta^2(t) \\ &\quad + \frac{2(T-2)}{(T-1)^2}\sum_{t\neq t'} r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')} \\ &\quad + \frac{T-2}{T-1}\left[\sum_{i=1}^{T}\sum_{t=1}^{T}\{R_i(t)-\bar{R}_i(\cdot)\}^2 + \sum_{j=1}^{T}\sum_{t=1}^{T}\{C_j(t)-\bar{C}_j(\cdot)\}^2\right].\end{aligned}$$

From before, we have

$$\begin{aligned}\mathbb{E}\{(T-1)S_1^2\} &= T\sum_{t=1}^{T}\mathrm{Var}\{\bar{x}_{\cdot\cdot}^o(t)\} - T^2\mathrm{Var}(\bar{y}_{\cdot\cdot}) + T\sum_{t=1}^{T}\{\bar{X}_{\cdot\cdot}(t)-\bar{X}_{\cdot\cdot}(\cdot)\}^2 \\ &= (T-1)\sigma_\epsilon^2 + \sum_{t=1}^{T}\sigma_\eta^2(t) + \frac{1}{(T-1)^2}\sum_{t\neq t'} r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')} \\ &\quad + T\sum_{t=1}^{T}\{\bar{X}_{\cdot\cdot}(t)-\bar{X}_{\cdot\cdot}(\cdot)\}^2.\end{aligned}$$

Thus, for LSs, the expected mean residual sum of squares is

$$\begin{aligned}\mathbb{E}(S_0^2) &= \sigma_\epsilon^2 + \frac{T-2}{(T-1)^2}\sum_{t=1}^{T}\sigma_\eta^2(t) + \frac{2}{(T-1)^3}\sum_{t\neq t'} r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')} \\ &\quad + \frac{1}{(T-1)^2}\left[\sum_{i=1}^{T}\sum_{t=1}^{T}\{R_i(t)-\bar{R}_i(\cdot)\}^2 + \sum_{j=1}^{T}\sum_{t=1}^{T}\{C_j(t)-\bar{C}_j(\cdot)\}^2\right],\end{aligned}$$

and the expected mean treatment sum of squares is

$$\mathbb{E}(S_1^2) = \sigma_\epsilon^2 + \frac{1}{T-1}\sum_{t=1}^{T}\sigma_\eta^2(t) + \frac{1}{(T-1)^3}\sum_{t\neq t'} r(t,t')\sqrt{\sigma_\eta^2(t)\sigma_\eta^2(t')} + \frac{T}{T-1}\sum_{t=1}^{T}\{\bar{X}_{\cdot\cdot}(t) - \bar{X}_{\cdot\cdot}(\cdot)\}^2.$$

A.3 Latin Square Probabilities

For the LS assignment mechanism, treatment labels are fixed and we randomly choose a LS of order T, with $T \in \mathbb{Z}_{\geq 3}$ a fixed integer.

Lemma A.3.1. *For any cell (i,j) and treatment t, there exists at least one LS with treatment t in (i,j).*

Proof. The Cayley table of the cyclic group $(\mathbb{Z}/T\mathbb{Z}, +)$ is a LS. Because treatment t appears in row i, switch two columns so that t is in cell (i,j). The transformed square is a LS. □

Lemma A.3.2. *The number of LSs with t' in cell (i,j) equals the number of LSs with t in cell (i,j), where $t \neq t'$.*

Proof. Consider two distinct LSs with treatment t in cell (i,j). In the interior of each square, relabel all the t cells as t' and all the t' cells as t. The transformed squares remain distinct LSs. Hence the number of LSs with t' in cell (i,j) is greater than or equal to the number of LSs with t in (i,j), and so by symmetry must be equal. □

Corollary A.3.3. *For $t \neq t'$, $\Pr\{W_{ij}(t) = 1\} = \Pr\{W_{ij}(t') = 1\}$.*

Proposition A.3.4. *For any cell (i, j) and treatment t,* $\Pr\{W_{ij}(t) = 1\} = 1/T$.

Proof. From the definition of a LS,

$$1 = \sum_{t=1}^{T} \Pr\{W_{ij}(t) = 1\} = T\Pr\{W_{ij}(1) = 1\}$$

$$\Rightarrow \Pr\{W_{ij}(t) = 1\} = \frac{1}{T} \; \forall t \in \{1, \ldots, T\}.$$

□

We now calculate probabilities for distinct cells. From the definition of a LS,

$$\Pr\{W_{ij}(t) = W_{ij'}(t) = 1\} = \Pr\{W_{ij}(t) = W_{i'j}(t) = 1\} = 0$$

for $i \neq i', j \neq j'$. First are probabilities for cells in the same row/column with different treatments.

Lemma A.3.5. *The number of LSs with t in (i, j) and t' in (i, j') equals the number of LSs with t in (i, j) and t'' in (i, j'), where $t, t', t'' \in \{1, \ldots, T\}$ are all distinct and $j \neq j'$.*

Proof. For any two distinct LSs with t in (i, j) and t' in (i, j'), relabeling all the t' as t'' and all the t'' as t' in their interiors yields two distinct LSs with t in (i, j) and t'' in (i, j'). This lemma follows by symmetry. □

Lemma A.3.6. *The number of LSs with t in (i, j) and t' in (i, j') equals the number of LSs with t' in (i, j) and t in (i, j'), where $t \neq t', j \neq j'$.*

Proof. For any two distinct LSs with t in (i, j) and t' in (i, j'), relabeling all the t' as t and all the t as t' in their interiors yields two distinct LSs with t' in (i, j) and t in (i, j'). This lemma follows by symmetry. □

Corollary A.3.7. *For $j \neq j'$, $\Pr\{W_{ij}(t) = W_{ij'}(t') = 1\}$ is constant as a function of (distinct) $t, t' \in \{1, \ldots, T\}$.*

Proposition A.3.8. *For $j \neq j', t \neq t'$, $\Pr\{W_{ij}(t) = W_{ij'}(t') = 1\} = 1/\{T(T-1)\}$.*

Proof. From the definition of a LS, the probability of two different treatments being assigned to (i, j) and (i, j') is equal to 1. Hence

$$1 = \sum_{t=1}^{T} \sum_{t \neq t'} \Pr\{W_{ij}(t) = W_{ij'}(t') = 1\} = T(T-1)\Pr\{W_{ij}(1) = W_{ij'}(2) = 1\}$$

$$\Rightarrow \Pr\{W_{ij}(t) = W_{ij'}(t') = 1\} = \frac{1}{T(T-1)} \; \forall t \neq t'.$$

□

By symmetry, we obtain the following.

Proposition A.3.9. *For $i \neq i', t \neq t'$, $\Pr\{W_{ij}(t) = W_{i'j}(t') = 1\} = 1/\{T(T-1)\}$.*

We now consider different rows and columns with the same treatments.

Lemma A.3.10. *For distinct cells $(i_1, j_1), \ldots, (i_T, j_T)$, with $i_1, \ldots, i_T \in \{1, \ldots, T\}$ all distinct and $j_1, \ldots, j_T \in \{1, \ldots, T\}$ all distinct, there exists at least one LS with treatment t in all these cells.*

Proof. The Cayley table of the cyclic group $(\mathbb{Z}/T\mathbb{Z}, +)$ is a LS. For each row in this LS, switch two columns to ensure that t is in all the cells $(i_1, j_1), \ldots, (i_T, j_T)$, which can be done as each treatment occurs only once in any row and column. □

Lemma A.3.11. *The number of LSs with t in all of $(i_1, j_1), \ldots, (i_T, j_T)$ equals the number of LSs with t in all of $(i'_1, j'_1), \ldots, (i'_T, j'_T)$, where $i_1, \ldots, i_T$ are distinct, $j_1, \ldots, j_T$ are distinct, and similarly $i'_1, \ldots, i'_T$ are distinct, $j'_1, \ldots, j'_T$ are distinct.*

Proof. For any two distinct LSs with t in all of $(i_1, j_1), \ldots, (i_T, j_T)$, simply switch the required columns in the desired order to obtain two distinct LSs with t in all of $(i'_1, j'_1), \ldots, (i'_T, j'_T)$. This lemma then follows by symmetry. □

Corollary A.3.12. *For any T cells $(i_1, j_1), \ldots, (i_T, j_T)$, with $i_1, \ldots, i_T$ all distinct and $j_1, \ldots, j_T$ all distinct,* $\Pr\{W_{i_1 j_1}(t) = \ldots = W_{i_T j_T}(t) = 1\} = 1/T!$.

Proof. From the definition of a LS, the probability that treatment t is in T distinct cells is equal to 1. Taking into account the $T!$ possible permutations of the columns of distinct cells and the results above,

$$T! \times \Pr\{W_{i_1 j_1}(t) = \ldots = W_{i_T j_T}(t) = 1\} = 1$$

$$\Rightarrow \Pr\{W_{i_1 j_1}(t) = \ldots = W_{i_T j_T}(t) = 1\} = \frac{1}{T!}.$$

□

Proposition A.3.13. *For $i_1 \neq i_2, j_1 \neq j_2$,* $\Pr\{W_{i_1 j_1}(t) = W_{i_2 j_2}(t) = 1\} = 1/\{T(T-1)\}$.

Proof.

$$\begin{aligned}\Pr\{W_{i_1 j_1}(t) = W_{i_2 j_2}(t) = 1\} &= \sum_{(i_3, j_3), \ldots, (i_T, j_T)} \Pr\{W_{i_1 j_1}(t) = \ldots = W_{i_T j_T}(t) = 1\} \\ &= \frac{(T-2)!}{T!}\end{aligned}$$

□

We finally consider different rows and columns with different treatments.

Lemma A.3.14. *The number of LSs with t in (i,j) and t' in (i',j') equals the number of LSs with t in (i,j) and t'' in (i',j'), and equals the number of LSs with t' in (i,j) and t in (i',j'), where $i \neq i', j \neq j'$, and t, t', t'' are distinct.*

Proof. This follows by the same reasoning as before. □

Corollary A.3.15. *For $i \neq i', j \neq j'$, and distinct t, t', t'',* $\Pr\{W_{ij}(t) = W_{i'j'}(t') = 1\} = \Pr\{W_{ij}(t) = W_{i'j'}(t'') = 1\} = \Pr\{W_{ij}(t') = W_{i'j'}(t) = 1\}$.

Proposition A.3.16. *For $i \neq i', j \neq j', t \neq t'$,* $\Pr\{W_{ij}(t) = W_{i'j'}(t') = 1\} = (T-2)/\{T(T-1)^2\}$.

Proof. From the definition of a LS, and our previous results,

$$
\begin{aligned}
1 &= \Pr[W_{ij}(t) = W_{i'j'}(t') = 1 \text{ for some } t, t' \in \{1, \ldots, T\}] \\
&= \sum_{t=1}^{T} \sum_{t'=1}^{T} \Pr\{W_{ij}(t) = W_{i'j'}(t') = 1\} \\
&= \frac{T}{T(T-1)} + T(T-1)\Pr\{W_{ij}(1) = W_{i'j'}(2) = 1\} \\
&\Rightarrow \Pr\{W_{ij}(t) = W_{i'j'}(t') = 1\} = \frac{T-2}{T(T-1)^2} \ \forall t \neq t'.
\end{aligned}
$$

□

Appendix B

Supplementary Materials for Chapter 2

B.1 An Additional Operation for Further Simplification of Proofs

For factors A_1, A_2, define $A_1 \odot A_2 = (b_{12,\mathrm{LL}}, b_{12,\mathrm{LQ}})'$, $A_1^2 \odot A_2 = (b_{12,\mathrm{QL}}, b_{12,\mathrm{QQ}})'$. Here, $A_1 \odot A_2$ and $A_1^2 \odot A_2$ divide $A_1 \otimes A_2$ by whether A_1 has a linear or quadratic effect, so that $A_1 \otimes A_2 = (A_1 \odot A_2,\ A_1^2 \odot A_2)'$. Sequential application of $\otimes$ and $\odot$ is defined in the manner below:

$$\begin{aligned} A_1 \odot (A_2 \otimes A_3) &= (b_{123,\mathrm{LLL}}, b_{123,\mathrm{LLQ}}, b_{123,\mathrm{LQL}}, b_{123,\mathrm{LQQ}})', \\ A_1^2 \odot (A_2 \otimes A_3) &= (b_{123,\mathrm{QLL}}, b_{123,\mathrm{QLQ}}, b_{123,\mathrm{QQL}}, b_{123,\mathrm{QQQ}})'. \end{aligned}$$

This is easily generalized to more factors, and provides another calculation in lieu of $\otimes$. For example, for factors A_1, A_2, A_3 forming an orthogonal array of strength two:

$$A_1 \odot (A_2 \otimes A_3) = 2^{-3}3^{3-s}\left\{\bigotimes_{j=1}^{2}\begin{pmatrix}1 & -1\\ 1 & 1\end{pmatrix}\right\}\left(\sum_{x\in\mathcal{F}_{23,\mathrm{LL}}} X_{1,\mathrm{L}}(x), \sum_{x\in\mathcal{F}_{23,\mathrm{LQ}}} X_{1,\mathrm{L}}(x), \sum_{x\in\mathcal{F}_{23,\mathrm{QL}}} X_{1,\mathrm{L}}(x), \sum_{x\in\mathcal{F}_{23,\mathrm{QQ}}} X_{1,\mathrm{L}}(x)\right)', \quad \text{(B.1.1)}$$

$$A_1^2 \odot (A_2 \otimes A_3) = 2^{-3}3^{3-s}\left\{\bigotimes_{j=1}^{2}\begin{pmatrix}1 & -1\\ 1 & 1\end{pmatrix}\right\}\left(\sum_{x\in\mathcal{F}_{23,\mathrm{LL}}} X_{1,\mathrm{L}}(x)^2, \sum_{x\in\mathcal{F}_{23,\mathrm{LQ}}} X_{1,\mathrm{L}}(x)^2, \sum_{x\in\mathcal{F}_{23,\mathrm{QL}}} X_{1,\mathrm{L}}(x)^2, \sum_{x\in\mathcal{F}_{23,\mathrm{QQ}}} X_{1,\mathrm{L}}(x)^2\right)' \quad \text{(B.1.2)}$$

$$- (0, 0, 0, b_{\phi,\phi})'.$$

B.2 Proofs

Proof of Proposition 2.3.1. First consider the proof of (2.3.1), with $k > j + 1$. The indicator function for $\mathcal{F}$ is

$$F(x) = \sum_{I\in\mathcal{P}}\sum_{T\in\mathcal{T}_I} b_{I,T}X_{I,T}(x),$$

and so

$$\sum_{x\in\mathcal{F}} X_{i_1,\mathrm{L}}(x)\cdots X_{i_j,\mathrm{L}}(x)X_{i_{j+1},\mathrm{L}}(x)^2X_{i_{j+1},\mathrm{Q}}(x)\cdots X_{i_k,\mathrm{L}}(x)^2X_{i_k,\mathrm{Q}}(x)$$

is written as

$$\sum_{x\in\mathcal{D}}\sum_{I\in\mathcal{P}}\sum_{T\in\mathcal{T}_I} b_{I,T}X_{I,T}(x)X_{i_1,\mathrm{L}}(x)\cdots X_{i_j,\mathrm{L}}(x)X_{i_{j+1},\mathrm{L}}(x)^2X_{i_{j+1},\mathrm{Q}}(x)\cdots X_{i_k,\mathrm{L}}(x)^2X_{i_k,\mathrm{Q}}(x).$$

Recalling Lemma 2.2.1 and noting that $X_{i,\mathrm{L}}(x) = 0$ when $X_{i,\mathrm{Q}}(x) = -2$, and $X_{i,\mathrm{Q}}(x) = 1$ when $X_{i,\mathrm{L}}(x) = \pm 1$, the expression immediately above is rewritten as

$$b_{i_1\cdots i_k,T_1\cdots T_k}\sum_{x\in\mathcal{D}} X_{i_1,\mathrm{L}}(x)^2\cdots X_{i_k,\mathrm{L}}(x)^2 + b_{i_1\cdots i_j,T_1\cdots T_j}\sum_{x\in\mathcal{D}} X_{i_1,\mathrm{L}}(x)^2\cdots X_{i_k,\mathrm{L}}(x)^2$$
$$+\sum_{m=1}^{k-j-1}\sum_{\substack{l_1,\ldots,l_m\in\{j+1,\ldots,k\}:\\ l_1<\cdots<l_m}}\left\{b_{i_1\cdots i_j i_{l_1}\cdots i_{l_m},T_1\cdots T_j T_{l_1}\cdots T_{l_m}}\sum_{x\in\mathcal{D}} X_{i_1,\mathrm{L}}(x)^2\cdots X_{i_k,\mathrm{L}}(x)^2\right\}.$$

This expression is simplified by using the fact that $\sum_{x\in\mathcal{D}} X_{i_1,\mathrm{L}}(x)^2\cdots X_{i_k,\mathrm{L}}(x)^2 = 2^k 3^{s-k}$. The remainder of the proposition is proved in a similar fashion. □

Lemma B.2.1. *For an* $\mathrm{OA}(9,s,3,2)$, $|b_{123,\mathrm{LLQ}}| = |b_{123,\mathrm{LQL}}| = |b_{123,\mathrm{QLL}}|$ *and* $|b_{123,\mathrm{LQQ}}| = |b_{123,\mathrm{QLQ}}| = |b_{123,\mathrm{QQL}}|$.

Proof. An $\mathrm{OA}(9,3,3,2)$ is a Latin square. Computing $b_{123,\mathrm{LLQ}}, b_{123,\mathrm{LQL}}$, and $b_{123,\mathrm{QLL}}$ for each of the 12 Latin squares of order 3, it follows that $|b_{123,\mathrm{LLQ}}| = |b_{123,\mathrm{LQL}}| = |b_{123,\mathrm{QLL}}|$. The other relationships are similarly established. Thus the result is true for $\mathrm{OA}(9,3,3,2)$, and because the projection of an $\mathrm{OA}(9,s,3,2)$ on any 3 factors is a Latin square, the result holds for any $s > 2$. □

Proof of Proposition 2.4.1. From Lemma B.2.1, this holds for $n = 2$. Assume it is true for $n = m$, where $m \geq 2$. Then consider $m+2$ factors $A_1,\ldots,A_{m+2}$ in an orthogonal array $\mathcal{F}$ of strength $m+1$ with 3^{m+1} runs. We see that

$$\sum_{x\in\mathcal{F}} X_{1,\mathrm{L}}(x)\cdots X_{m+1,\mathrm{L}}(x)X_{m+2,\mathrm{L}}(x)^2 = \sum_{x\in\mathcal{F}_{1,\mathrm{L}}} X_{2,\mathrm{L}}(x)\cdots X_{m+1,\mathrm{L}}(x)X_{m+2,\mathrm{L}}(x)^2$$
$$-\sum_{x\in\mathcal{F}_{1,\mathrm{Q}}} X_{2,\mathrm{L}}(x)\cdots X_{m+1,\mathrm{L}}(x)X_{m+2,\mathrm{L}}(x)^2.$$

As $\mathcal{F}$ is an orthogonal array of strength $m+1$, for all $x \in \mathcal{F}_{1,\mathrm{L}}$, any m factors chosen from $A_2, \ldots, A_{m+2}$ form an orthogonal array of strength m and 3^m runs. The same statement holds true for all $x \in \mathcal{F}_{1,\mathrm{Q}}$. By the inductive hypothesis, we have

$$\sum_{x \in \mathcal{F}_{1,\mathrm{L}}} X_{2,\mathrm{L}}(x) \cdots X_{m+1,\mathrm{L}}(x) X_{m+2,\mathrm{L}}(x)^2 = \pm \sum_{x \in \mathcal{F}_{1,\mathrm{L}}} X_{2,\mathrm{L}}(x) \cdots X_{m+1,\mathrm{L}}(x)^2 X_{m+2,\mathrm{L}}(x),$$

$$-\sum_{x \in \mathcal{F}_{1,\mathrm{Q}}} X_{2,\mathrm{L}}(x) \cdots X_{m+1,\mathrm{L}}(x) X_{m+2,\mathrm{L}}(x)^2 = \mp \sum_{x \in \mathcal{F}_{1,\mathrm{Q}}} X_{2,\mathrm{L}}(x) \cdots X_{m+1,\mathrm{L}}(x)^2 X_{m+2,\mathrm{L}}(x),$$

so that

$$\sum_{x \in \mathcal{F}} X_{1,\mathrm{L}}(x) \cdots X_{m+1,\mathrm{L}}(x) X_{m+2,\mathrm{L}}(x)^2 = \pm \sum_{x \in \mathcal{F}} X_{1,\mathrm{L}}(x) \cdots X_{m+1,\mathrm{L}}(x)^2 X_{m+2,\mathrm{L}}(x).$$

From Proposition 2.3.1, these equalities establish that $|b_{1\cdots(m+2),\mathrm{L}\cdots\mathrm{LQ}}| = |b_{1\cdots(m+2),\mathrm{L}\cdots\mathrm{QL}}|$. The other equalities follow similarly, thus completing the induction step. □

Lemma B.2.2. *For factors A_1, A_2, A_3, A_4 in an* $\mathrm{OA}(9, s, 3, 2)$, $A_1 \otimes A_2 \otimes A_3 \otimes A_4 = (0, \ldots, 0)'$.

Proof. The proof follows in a similar manner as that of Lemma B.2.1 by noting that the projection of the $\mathrm{OA}(9, s, 3, 2)$ on any four factors is a Graeco-Latin square, and applying Proposition 2.3.1. □

Proof of Proposition 2.4.3. A similar induction argument as in Proposition 2.4.1, combined with Lemma B.2.2 and the relations among the indicator function coefficients given in Proposition 2.3.1, yields the result. □

Proof of Proposition 2.5.1. The first statement follows from (B.1.1) and the fact that

the Hadamard matrix in this equation is non-singular. To prove the second, $A_3^2 \odot (A_1 \otimes A_2)$ in (B.1.2) is written as

$$2^{-3}3^{3-s}\left\{\bigotimes_{j=1}^{2}\begin{pmatrix}1 & -1\\ 1 & 1\end{pmatrix}\right\}\left\{\begin{pmatrix}\sum_{x\in\mathcal{F}_{12,\mathrm{LL}}} X_{3,\mathrm{L}}(x)^2\\ \sum_{x\in\mathcal{F}_{12,\mathrm{LQ}}} X_{3,\mathrm{L}}(x)^2\\ \sum_{x\in\mathcal{F}_{12,\mathrm{QL}}} X_{3,\mathrm{L}}(x)^2\\ \sum_{x\in\mathcal{F}_{12,\mathrm{QQ}}} X_{3,\mathrm{L}}(x)^2\end{pmatrix} - 2^1 3^{s-3}\begin{pmatrix}\frac{k}{3^{s-2}}\\ \frac{k}{3^{s-2}}\\ \frac{k}{3^{s-2}}\\ \frac{k}{3^{s-2}}\end{pmatrix}\right\},$$

where $k = |\mathcal{F}|/9$. The expression above is $(0,\ldots,0)'$ if and only if

$$\sum_{x\in\mathcal{F}_{12,\mathrm{LL}}} X_{3,\mathrm{L}}(x)^2 = \sum_{x\in\mathcal{F}_{12,\mathrm{LQ}}} X_{3,\mathrm{L}}(x)^2 = \sum_{x\in\mathcal{F}_{12,\mathrm{QL}}} X_{3,\mathrm{L}}(x)^2 = \sum_{x\in\mathcal{F}_{12,\mathrm{QQ}}} X_{3,\mathrm{L}}(x)^2 = \frac{2k}{3},$$

which is impossible if k is not divisible by 3. □

Proof of Proposition 2.5.4. First, note that for $a_1,\ldots,a_n,a_{n+2}\in\{1,2\}$,

$$\sum_{x\in\mathcal{F}} X_{1,\mathrm{L}}(x)^{a_1}\cdots X_{n,\mathrm{L}}(x)^{a_n} X_{n+1,\mathrm{L}}(x) X_{n+2,\mathrm{L}}(x)^{a_{n+2}} =$$

$$\sum_{x\in\mathcal{F}_{n+1,\mathrm{L}}} X_{1,\mathrm{L}}(x)^{a_1}\cdots X_{n,\mathrm{L}}(x)^{a_n} X_{n+2,\mathrm{L}}(x)^{a_{n+2}} - \sum_{x\in\mathcal{F}_{n+1,\mathrm{Q}}} X_{1,\mathrm{L}}(x)^{a_1}\cdots X_{n,\mathrm{L}}(x)^{a_n} X_{n+2,\mathrm{L}}(x)^{a_{n+2}}.$$

As $A_1,\ldots,A_n,A_{n+1}$ form an orthogonal array of strength $n+1$, the expression above is zero, and so by Proposition 2.3.1, $A_{n+1}\odot(A_1\otimes\cdots\otimes A_n\otimes A_{n+2}) = (0,\ldots,0)'$. A similar reasoning leads to $A_{n+1}^2\odot(A_1\otimes\cdots\otimes A_n\otimes A_{n+2}) = (0,\ldots,0)'$, establishing the proposition. □

Appendix C

Supplementary Materials for Chapter 3

C.1 Correlation in ϵ

In all our analyses, we assumed the ϵ_i were independent. As pointed out by a referee, when units reside on a constrained boundary, independence of error terms is not generally a realistic assumption. However, we believe that our specific context helps justify this simplifying assumption for several reasons.

First, the major objective driving our work on 3D printing is compensation for product deformation. To derive compensation plans, it is important to accurately specify the mean trend in deformation. Although incorporating correlation may change parameter estimates that govern the mean trend, we do not believe that modeling the correlation in errors will substantially help us compensate for printed product deformations. This is something we intend to address further in our future

work.

Second, there is a factor that may further confound the potential benefits of including correlated errors in our model: the resolution of the CAD model. To illustrate, consider the model fit in Section 3.3.1. We display the residual plots below. All residuals are (in absolute value) less than 1% of the nominal radius for $r_0 = 0.5$ inch, and at most approximately 0.1% of the nominal radius for $r_0 = 1, 2, 3$ inches, supporting our claim that we have accurately modeled the mean trend in deformation for these products. However, we note that for $r_0 = 1, 2, 3$ inches, there is substantial negative correlation in residuals between adjacent units, with the residuals following a high-frequency harmonic trend. There is a simple reason driving this phenomenon. Our first manufactured products were $r_0 = 1, 2, 3$ inches, and the CAD models for these products had low resolution. Low resolution in the CAD model yields the high-frequency pattern in the residual plots. The next product we constructed was $r_0 = 0.5$ inch, and its CAD model had higher resolution than that previously used, which helped to remove this high-frequency pattern. Minor trends appear to exist in this particular plot, and an ACF plot formally reveals significant autocorrelations. Accordingly, we observe that the correlation in residuals is a function of the resolution of the initial CAD model. In consideration of our current data, and our primary objective to accurately capture the mean trend in deformation, we use independent ϵ_i throughout. We intend to pursue this issue further in our future work, for example, in the direction of Colosimo, Semeraro, and Pacella (2008).

Furthermore, as pointed out by the Associate Editor, correlations in residuals for more complicated products may be accounted for by modeling the interference

between units, and the issue of interference is precisely the focus of this manuscript.

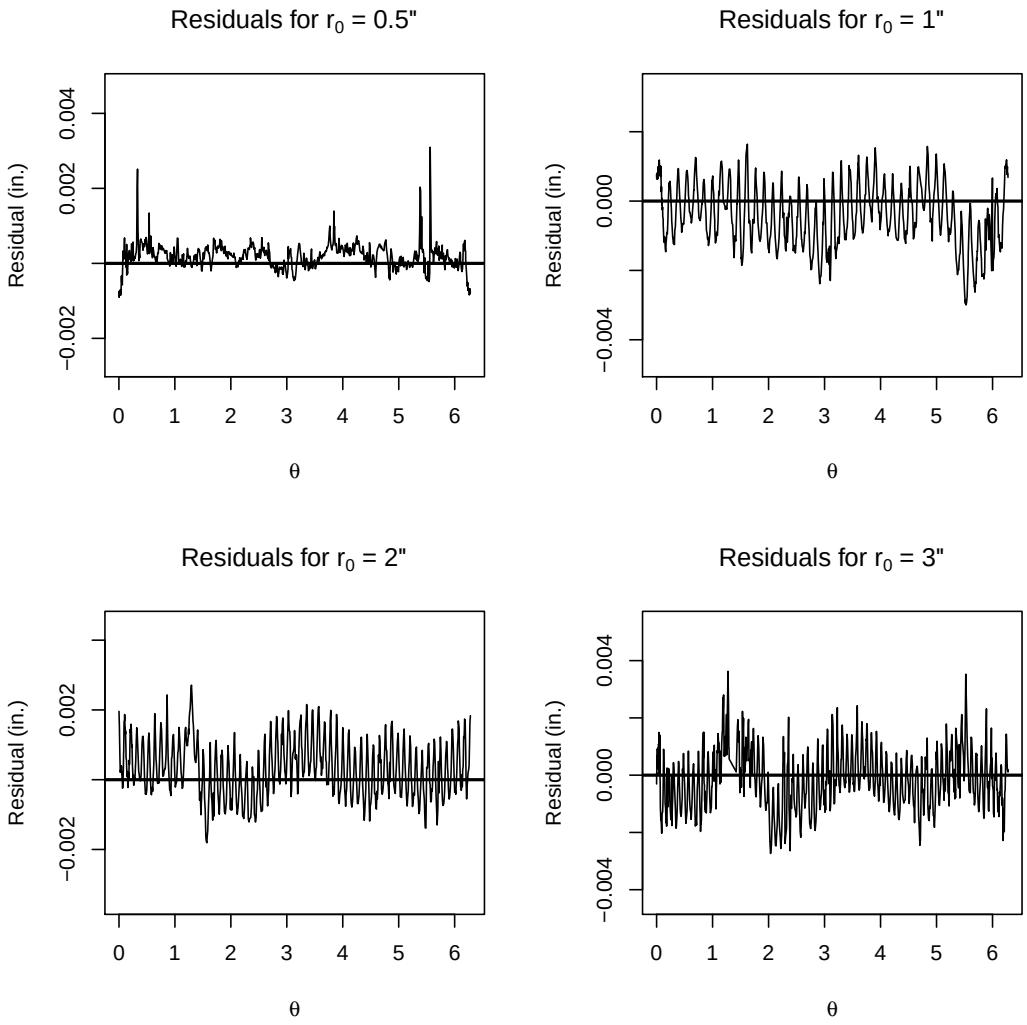

Figure C.1: Residuals for the model fit in Section 3.3.1. Here, the residual is defined as the difference between the observed deformation and the posterior mean of deformation for each angle θ_i.

C.2 MCMC Convergence Diagnostics

Convergence of our MCMC algorithms was gauged by analysis of ACF and trace plots, and effective sample size (ESS) and Gelman and Rubin (GR, 1992) statistics, which were calculated using 10 independent chains of 1000 draws after a burn-in of 500. In Sections 3.3.1 and 3.3.4, the ESS were all above 8000 (the maximum is 10000), and the GR statistics were all 1.

C.3 Assessing Interference

The results of the first procedure described in Section 3.3.3 are displayed in Figure C.2: bold lines represent posterior means, dashed lines quantiles forming the 99% central posterior intervals, and dots the observed outcomes in the experiment, with separate figures for each nominal radius and compensation. For example, the graph in the first row and column of Figure C.2 contains the observed data for angles in the 0.5 inch radius cylinder that received -1 compensation. This figure also contains the posterior predictive mean and 99% intervals for all angles under the assumption that -1 compensation was applied uniformly to the cylinder. Although only four sections of the cylinder received this compensation in the experiment, forming this distribution makes the posterior predictive mean trend transparent, and so helps identify when a unit's observed outcome deviates strongly from its prediction.

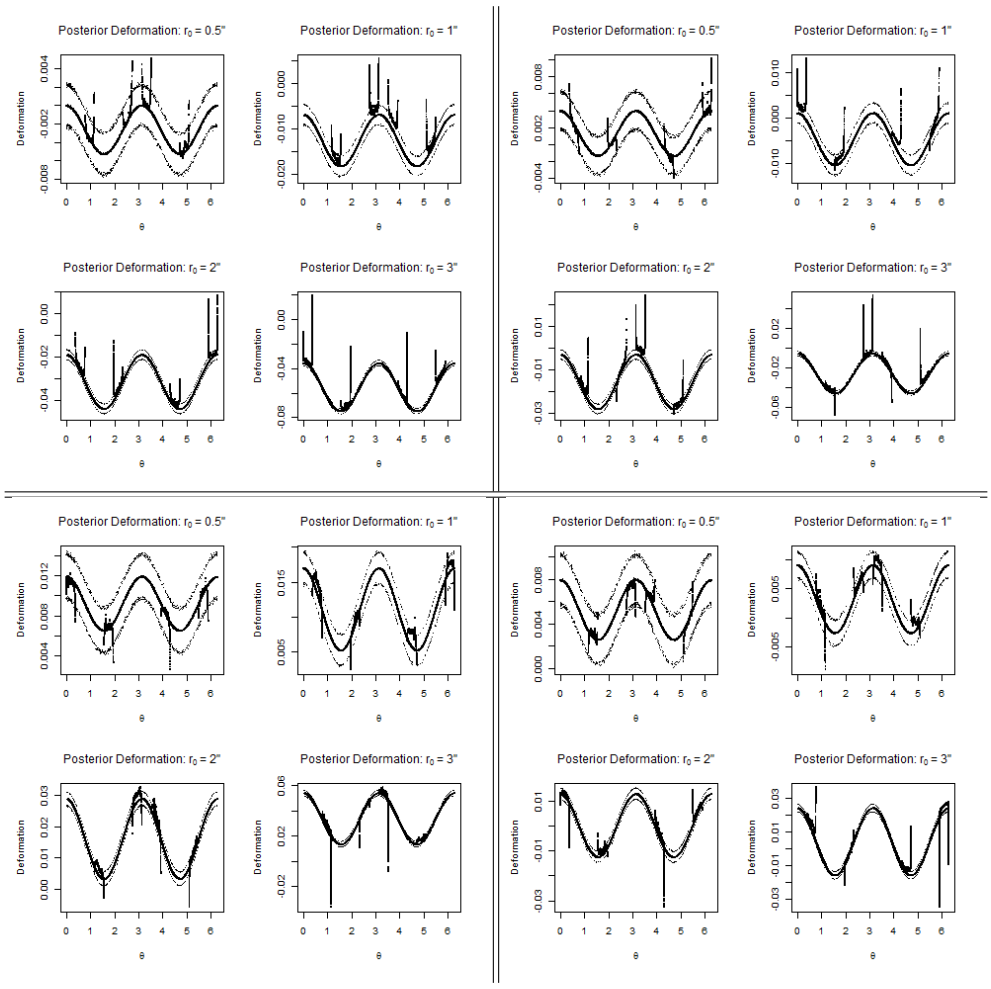

Figure C.2: Assessing interference in the experiment based on posterior inferences drawn from the no-compensation data. Clockwise from top left: predictions for units that received $-1, 0, +1$, and $+2$ compensation.

C.4 Note on a Class of Interference Models

Compensation is applied in practice by discretizing the plan at a finite number of points, according to some tolerance specified by the size (in radians) for each section, or alternatively the maximum value of $|\theta_{i,M} - \theta_{i,NM}|$.

Suppose compensation plan $x(\theta)$ is a continuous function of θ, and define

$$w_i = \frac{h(|\theta_i - \theta_{i,M}|)}{h(|\theta_i - \theta_{i,M}|) + h(|\theta_i - \theta_{i,NM}|)},$$

with $h : \mathbb{R} \to \mathbb{R}_{>0}$ a monotonically decreasing continuous function, and

$$g_i(\mathbf{x}) = w_i x_{i,M} + (1 - w_i) x_{i,NM}.$$

Then for the cylinder product considered in our experiment, $g_i(\mathbf{x}) \to x_i$ as $|\theta_{i,M} - \theta_{i,NM}| \to 0$. To show this, we first recognize that $|x_{i,M} - x_{i,NM}| \to 0$ as $|\theta_{i,M} - \theta_{i,NM}| \to 0$. Therefore, as

$$0 \leq |\theta_i - \theta_{i,NM}| - |\theta_i - \theta_{i,M}| \leq |\theta_{i,M} - \theta_{i,NM}|,$$

$g_i(\mathbf{x}) \to x_i$ as $|\theta_{i,M} - \theta_{i,NM}| \to 0$.

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